

PLANNING STUDY FOR ADVANCED NATIONAL
SYNCHROTRON-RADIATION FACILITIES

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The report of a study sponsored by the Department of Energy,
Office of Basic Energy Sciences, and co-chaired by
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A new generation of synchrotron-radiation sources based on insertion devices offers gains in photon-beam brilliance as large as the gains that present-day synchrotron sources provided over conventional sources. This revolution in synchrotron capability and its impact on science and technology will be as significant as the original introduction of synchrotron radiation. This report recommends that insertion-device technology be pursued as our highest priority, both through the full development of insertion-device potential on existing machines and through the building of new facilities.

PREFACE

This report presents the results of a study by an ad hoc committee sponsored by the Department of Energy (DOE), Office of Basic Energy Sciences, with the charter to "solicit and evaluate ideas from synchrotron-radiation providers and users as to the future opportunities and technical needs for synchrotron-radiation based research." The committee was further charged "to establish from the available options a set of priorities for the timely development of both existing and new facilities that can meet those needs."

This study critically evaluates the current status and opportunities for synchrotron radiation (SR)-based science and technology, facilities, and users. The evaluation serves as the basis for a series of recommendations for SR that includes upgrading of existing facilities, new instrumentation, new facilities, and methods of increasing user participation. While the focus of the report is a series of recommended actions, it also contains data, analyses, observations, and criticisms, so that it can serve as a resource for future deliberations.

Judgement Criteria

Our judgements were based generally on the new science and technology offered by the next generation of machines and specifically on the way in which the properties of new sources lead to new experimental capabilities. Our analysis took into account the technological barriers that define the limits of SR sources and various issues affecting the use of these sources by the scientific community.

Methodology

The objective of conducting a comprehensive and critical scientific review influenced the choice of the committee members and the procedures adopted to obtain and evaluate the needed information. The committee membership of seventeen, listed at the end of this preface, was drawn from universities, industry, and DOE and Department of Defense (DOD) laboratories. These members represent a wide range of disciplines and include 12 SR users.

To further broaden the representation, we solicited the testimony and active participation of many other scientists, including the personnel of facilities involved in providing SR. The breadth and sophistication of SR-based science and technology required the participation of all these people, and we thank them for their responsiveness and assistance.

Information was first obtained at a meeting held at Sandia National Laboratories, Albuquerque on October 8 and 9, 1983. Approximately 30 speakers and 80 participants gave testimony on science opportunities, facility needs, user needs, and plans for new facilities, including the proposal for the Berkeley Advanced Light Source (ALS), which we were specifically asked to examine. Over 1000 pages of written technical information was provided to the committee, much of which has been distilled and included in this report. The meeting included special sessions for debate and criticism.

As the study proceeded, the committee issued additional calls for letters of opinion from the community and for technical and factual information necessary in our deliberations. Over a hundred such correspondences were received from a broad range of scientific, technical, and institutional interests. Their input has been evaluated, distilled, and, where appropriate, included in this report.

The committee then met in executive session three times over the next three months, at Stanford, MIT, and Exxon, to evaluate the material it had received, to reach its major conclusions concerning the priorities for SR, and to prepare the report. On November 15, 1983, in response to a request from DOE, an interim version of the major conclusions and recommendations was submitted to DOE in the form of a letter, which is included as Appendix A.

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EXECUTIVE SUMMARY

Introduction

Throughout the development of modern science and technology, electromagnetic radiation has been the most effective of exploratory probes for the discovery of structural characteristics and for the understanding of physical processes. Success in such discoveries has been intimately linked to evolution and revolution in the technology of photon generation. The electric light, the discharge lamp, the x-ray tube, and the laser each ushered in new eras of science. We can now add to this list the most versatile of sources: synchrotrons, or storage rings for the generation of synchrotron radiation (SR).

SR has the unique capability of providing radiation over eight decades of the electromagnetic spectrum, from 10^{-3} to 10^5 eV. Thus, it reaches from the infrared, the visible, and the ultraviolet, through the soft and hard x-ray domains, and up to the gamma-ray region. Within the last few years we have become confident that SR facilities can be built that will provide unprecedented control of all the important characteristics of a photon beam: source size, spatial coherence, temporal coherence, spectral range, polarization, and time structure. As a source of electromagnetic radiation, only lasers and perhaps plasma sources will maintain any superiority for specific applications.

In the brief history of experimentation in the newly emerging field of SR science and scientific measurements, there are already significant accomplishments in a wide variety of fields. In solid state physics and in surface science, bulk and surface electronic structures have been measured. Grain boundaries and interfaces of important semiconductors and metals have been studied. Surface

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bond lengths have been determined to a degree of resolution that is important to the study of surface chemistry. In phase-transition physics, the first studies of structural transitions in two-dimensional systems have revealed new phases and new transition mechanisms. In biology, SR has been used to define the active site in important metalloenzymes like nitrogenase, the enzyme responsible for nitrogen fixation in plants. In energy research, the concentration and chemical state of impurities in coal and the structure of bimetallic catalysts have been determined. And in medicine, a noninvasive, low-dose angiography technique with the promise of wide applicability as a general medical imaging technique has been developed. Although some of the techniques used in SR science have been used earlier with conventional photon sources, the brightness and tunability of SR has carried experiment and measurement far beyond the capabilities of the past.

Though the thrusts to date have concentrated in the basic sciences, technological applications of SR are beginning to emerge, as evidenced by recent SR studies of catalysis, medical imaging, submicron lithography for the computer industry, defect structures in solids, amorphous materials, alloy-structure determination, phase changes in solids, and applications to biological materials.

The SR field has had a similar impact in the industrialized countries of Europe and Asia. All of these countries expect the industrial and defense applications to grow rapidly in significance, and they all are building their array of SR facilities to handle the work. In some countries--West Germany, France, England, the Soviet Union, and Japan--there are SR facilities comparable to those in the USA, and these countries all have high-priority programs to advance their capabilities.

Opportunities have now been demonstrated for orders-of-magnitude improvement in SR capabilities through the use of special insertion devices called wigglers and undulators and of storage rings with improved characteristics; these innovations make it possible to enhance and optimize the radiation for specific studies. The gains are not only in the intensity of the radiation source but also in its optical qualities, which include extraordinary collimation and small source size, variable polarization, and extremely short pulse lengths. This added control will lead to experiments not previously possible.

One sees expanding horizons of experimentation in basic condensed-matter sciences, in materials science and technology, and in chemistry, biology, and medicine, in addition to increased usage of some of the past techniques with better capabilities. The added flexibility offered by higher-brilliance sources will greatly enhance the sophistication of our physical probes and make possible studies of smaller and more dilute samples and of weaker phenomena. The future offers x-ray holography, various microscopies, studies of low-energy excitations and time-dependent phenomena, the determination of the properties of very small particles, and new frontiers in atomic, molecular, and plasma studies.

To meet the challenges and opportunities in both scientific-research and technological applications of SR, facilities will be needed that are dedicated to the utilization of insertion devices and that are readily accessible to the whole spectrum of university, industry, and defense interests. New machines dedicated to the utilization of insertion devices, even if they are developed on the most expeditious schedule, will not have significant impact until the late 1980s or early 1990s. Therefore, our recommendations include the full development of existing insertion-device capability, in parallel with the construction of new facilities specifically designed for the use of these devices.

Recommendations and Conclusions

I. Existing Facilities and Projects

The committee recommends that steps be taken to ensure the timely completion of the commissioning of the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory and the Synchrotron Radiation Center (SRC) at Stoughton, Wisconsin. We are encouraged by the actions at NSLS and SRC since our initial letter to the Department of Energy (DOE). To optimize utilization of existing facilities, we recommend providing operations funding, so that such facilities can provide a maximum of beam time in a "user friendly" mode, and continued research funding, so that it will be possible to take full advantage of the facilities.

To realize the full potential of existing facilities, the committee recommends expeditious completion of currently approved projects to construct insertion-device beamlines: the NSLS Phase II project at Brookhaven Laboratory and the SSRL Enhanced Photon Flux Facility (SEPPF) project at the Stanford Synchrotron Radiation Laboratory (SSRL). The future construction of additional insertion-device-based beamlines at existing facilities is strongly recommended.

II. Major New Facilities

The committee believes that major new programs based on the utilization of insertion devices are of central importance for effective progress in materials-science, physics, biology, and chemistry research over the next decade. The committee is therefore unanimous in its recommendations, which follow in order of priority.

1. The design and construction of a high-energy storage ring capable of providing fundamental undulator radiation in the x-ray region of the spectrum up to 20 keV, with an early 1990s target date for full operation of the facility.

To achieve this objective, appropriate research and development funding should be allocated now.

2. The construction of a second, lower-energy ring capable of providing fundamental undulator radiation in the soft x-ray region of the spectrum up to 2.0 keV. This machine should also provide picosecond (ps) timing capabilities. The Advanced Light Source (ALS) is such a machine.

The committee strongly recommends that no action based on the second-priority recommendation interfere with the timely pursuit of the first-priority recommendation.

III. Alternative-Source Facilities

Free-electron-laser (FEL), ultraviolet (UV)-laser, and laser-heated-plasma sources promise to make important complementary contributions at the low-energy end of the spectrum. To provide a complete full-spectrum capability, these sources should be developed in as timely a fashion as possible by their respective technical communities and funding agencies. However, the committee concluded that in the foreseeable future SR will continue to be the premier source of radiation in the soft x-ray and x-ray regions.

IV. Other Comments and Conclusions

The Need for Two Machines and their Relative Priority -- The physics governing the performance of undulators dictates that a machine designed to produce x-ray radiation at energies above 10 keV operate at a different energy level than a machine designed for the optimal production of soft x-ray ultraviolet (XUV) radiation at energies less than 2 keV. Using existing or anticipated technology, fundamental undulator radiation at 10 to 20 keV will require a 5 to 6-GeV machine, while optimized undulator radiation at less than 2 keV

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will require a machine operating at approximately 1.5 GeV. Factors governing the relative priority of these two machines include:

- A. There are no dedicated facilities where x-ray undulators can be developed, whereas some limited opportunities for developing XUV undulators do exist.
- B. Although the low-energy ring cannot provide undulator capability in the x-ray region, the high-energy machine can access some of the XUV region, albeit with reduced performance.

Commissioning of New Machines -- The difficulties being experienced in the commissioning of the newly constructed machines arise from overzealous attempts at economy, from some deficiencies in the project-management systems, and from a general lack of big-project experience in the materials-science community. These are not fundamental technical problems and should be rectified in future projects.

Improving Access to Facilities -- The access to SR facilities is currently being restricted by two major factors. The first factor is the difficulty experienced by university-based groups in obtaining the funding necessary for participation. We recommend that beamline funding at future and existing facilities be provided in such a way that university-based groups can participate more readily. This cooperation would significantly broaden both the technical base that could contribute to innovations in instrumentation and the scientific base that could contribute to effective use of the facility. A proposal-based, peer-reviewed approach for the selection of outside participants is strongly recommended.

The second factor is the limitation on the participation of industry, university, and government laboratories that are performing applied research. In deciding which groups can participate

in beamline usage, there is currently a bias towards fundamental research. The broadening of program-review committees to include applied interests, together with procedures to ensure more "user friendly" instrumentation and the protection of proprietary and classified interests, would increase the participation of applied-research groups.

Continuing Review -- The rapid developments in SR make it appropriate that a committee similar to ours convene periodically to review current developments in the entire field and to make recommendations for future actions.

SYNCHROTRON RADIATION

Introduction

Before synchrotron radiation (SR) was available for ultraviolet (UV) and x-ray experimentation, scientists relied on a collection of sources that had low intensity, lacked tunability, and in general did not provide radiation that was easily manipulated. The use of bending-magnet radiation from synchrotrons built for high-energy physics provided orders-of-magnitude increases in source intensity and brilliance and opened many research frontiers. The design of a new generation of dedicated machines (the National Synchrotron Light Source [NSLS] and the Synchrotron Radiation Center [SRC]) especially configured to produce a bright source is leading to further improvement. Now a new class of machines based not on bending-magnet radiation but on insertion devices promises increases in source brightness and quality as large as the original gains over conventional sources. It is this class of devices that has launched new initiatives for facility development. An understanding of the physics governing the performance of these new devices is necessary to appreciate the technical issues underlying the recommendations of this report. This section of the report provides the basic concepts needed for understanding the physics of insertion devices.

The Physics of Synchrotron Radiation

If the path of an ultrarelativistic electron of energy $E = \gamma mc^2$ (where m is the mass of the electron and c is the speed of light) is bent to a radius R by a magnetic field, it will emit radiation with a continuous (white) wavelength distribution centered around a critical wavelength

$$\lambda_c = R \gamma^{-3}. \quad (1)$$

The radiation is emitted into a narrow cone of opening angle

$$\delta = \gamma^{-1}. \quad (2)$$

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For $E = 3$ GeV and a typical bending radius of 20 meters, $\gamma = 6 \times 10^3$ and $\lambda = 1.0$ Å (approximately 12 keV), with an opening angle of 2×10^{-4} radians or about 40 seconds of arc. The radiation in the orbit plane is linearly polarized, and outside this plane it is elliptically polarized.

The brightness (intensity per unit solid angle and bandwidth) of such an x-ray source is 2 to 3 orders of magnitude greater than that of the characteristic lines of a modern 10-kW rotating-anode source; it is many more orders of magnitude more intense than the bremsstrahlung spectrum from such a source. Furthermore, the synchrotron source is continuously tunable, highly polarized, and directed into an extremely narrow beam. The radiation from an electron bunch comes in pulses as the electrons traverse the aperture of the beamline. For a typical single bunch, the repetition rate is on the order of hundreds of nanoseconds, and the pulse length is a small fraction of a nanosecond. This time structure has been found extremely useful in a wide variety of timing experiments. The Advanced Light Source (ALS) design would offer pulse lengths in the 10-ps range, opening a new regime for time-dependent studies.

Within the last 10 years, most SR-based experiments have been performed using whatever source characteristics the bending magnets of existing high-energy storage rings happened to have. Although the beams from these bending-magnet sources are considerably brighter than those obtained using conventional light sources, dramatic improvements are possible. The newest generation of storage rings (NSLS and SRC) has extremely small electron-beam cross section and angular divergence (i.e., low emittance), resulting in bending-magnet radiation with significantly higher source brilliance (brightness per unit source size). Even higher brilliances are possible using specially designed magnetic structures inserted in the straight sections of storage rings. The functional separation of the magnets that control the electron orbit and those that produce the radiation is an important strategic advantage allowing source design innovations to be implemented at will. The physics of these devices is described below.

Insertion Devices

A straight electron trajectory can be wiggled in a transverse magnetic field that is alternating, say N times, along the path in a device of length L . These insertion devices immediately provide an N -fold increase in intensity because the radiation from each of the N magnetic sources is superimposed in the forward direction. There are two different classes of insertion devices; the distinction between them depends on the strength of the orbit perturbation. If the electron path deviates by an angle that is approximately equal to or less than the opening angle of the SR, $1/\gamma$, then the device is called an undulator. Devices causing larger deviations are called wigglers. In addition to enhanced brilliance, other characteristics of the photon beam can be controlled by varying the magnetic period $\lambda_u = L/N$ and the strength of the magnetic field B . A key parameter determining performance is $K = 0.93 B(\text{TG})\lambda_u(\text{cm})$. To a first approximation, K is the ratio of the angular excursion of the electron to the synchrotron opening angle $1/\gamma$. If $K < 1$, the device is an undulator; for $K > 1$ it is a wiggler. The behavior of both these devices can be described by the same theory, but their properties can be significantly different. Both types have been tested and their behavior is in agreement with predictions. An $N = 27$, $K = 8$ wiggler at Stanford is currently the world's most powerful source of SR.

The total radiation produced by wigglers is similar to bending-magnet radiation in its vertical opening angle, $1/\gamma$, and its smooth spectral function. However, its horizontal opening angle is reduced to K/γ , and its intensity is multiplied by N . To understand the properties of undulators, one must take account of the interference of the radiation emitted by each of the $2N$ magnetic poles. This detailed interference theory is necessary as K decreases toward unity, but it is equally valid for high- K wigglers. The mathematical relationships that explain the precise properties of wigglers and undulators are contained in the footnotes below Figure 2. For the purposes of the following discussion, note that (1) undulator radiation has a structured spectrum consisting of peaks at the fundamental wavelength λ_p^1 and harmonics λ_p^m (Footnote 1), and (2) the fundamental radiation is emitted into a solid angle Ω (Footnote 2). With these definitions one can describe generally the performance of insertion devices. Figure 1 shows the spectral brilliance and the qualitative differences in the spatial character of the radiation from different sources. Spectra for two different undulators are depicted in Figure 2. Finally, Table 1 gives specific performance data for a number of different devices.

Generally, lower- K and higher- N devices (undulators) produce radiation with greater directionality. For a low- K undulator, the solid angle $\Omega = \frac{1}{\gamma^2 N}$, and it

contains a quasi-monochromatic beam with a fractional bandwidth $\Delta\lambda/\lambda$ equal to $1/N$. The total number of photons in this beam is increased by a factor of N and the brightness by a factor of N^2 , compared with a beam from a bending magnet. Typically, $N = 100$, so the gains are substantial. As shown by Footnote 4, the power in the fundamental P_1 is a substantial fraction (two thirds) of the total device power P_{TOT} when $K = 1$, and $P_1/P_{TOT} \rightarrow 1$ as $K \rightarrow 0$. Therefore, the most efficient production of radiation in a narrow bandwidth around λ_p occurs for devices with $K < 1$. As K increases with fixed λ_p and L (by varying either λ_1 or γ), the solid angle Ω remains constant. Thus, a high- K device is still capable of producing highly directional radiation of wavelength λ_p with N -fold intensity enhancement. However, this solid angle now includes substantial higher-harmonic power given by $\frac{K^2}{2} P_1$, and the bandwidth is increased to $(1 + K^2/2)/N$.

This decrease in coherence is a direct result of the large angular excursions of the electron in a high- K device, which diminish the relative range of angles over which constructive interference occurs.

Before discussing the specific consequences of the behavior described above for the next generation of machines, one more point should be made. The brilliance of $K = 1$ undulator beams is potentially so high that their ultimate quality is strongly dependent on the emittance of the storage ring. First, the spatial size of the electron beam in a storage ring must be small enough so that at a reasonable distance d one can select out an area $d^2\Omega$ through which the first harmonic will pass. Second, the angular divergence of the electron beam should be on the order of $\Omega^{1/2}$ or smaller. For this reason, the next generation of storage ring will be designed with very low emittance.

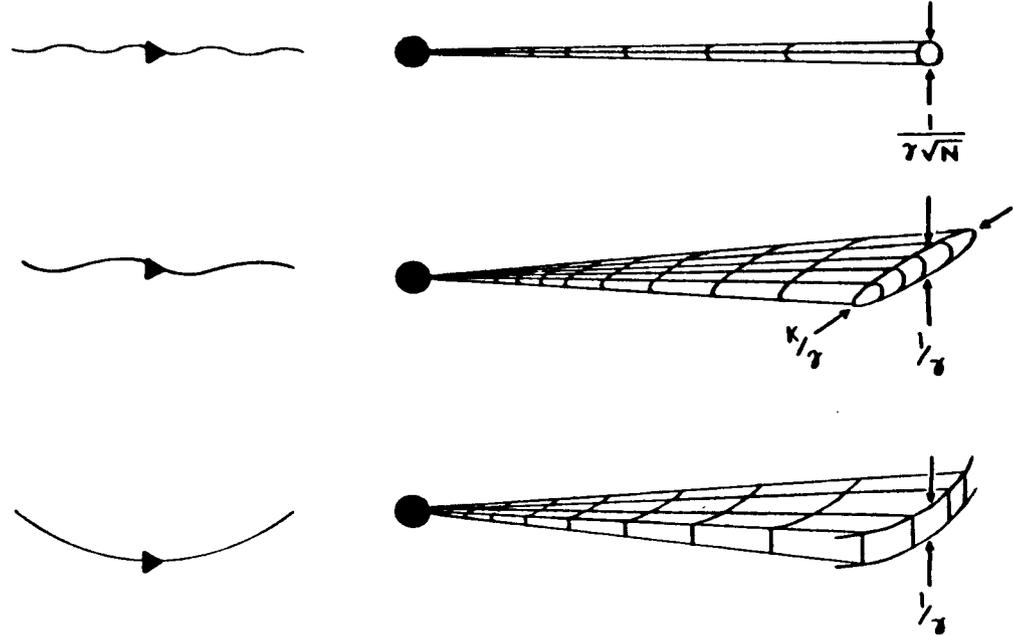
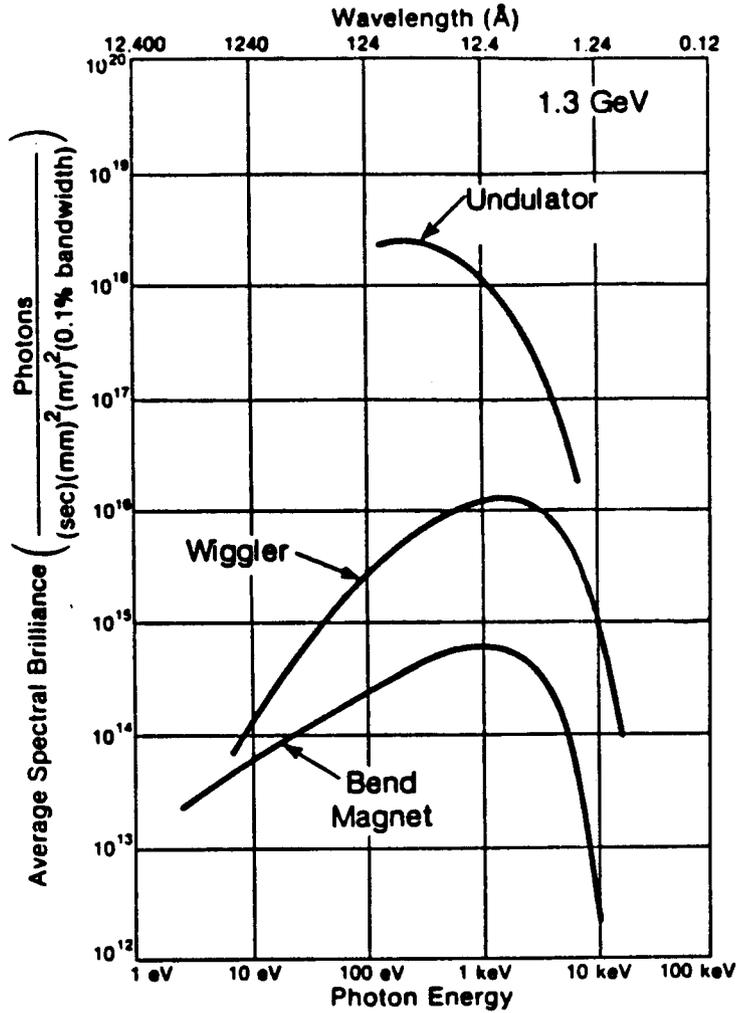


Figure 1. A Bending Magnet/Wiggler/Undulator Comparison. Left: The spectral brilliance as a function of photon energy for a bending magnet, wiggler, and undulator on a 1.3-GeV ring (the ALS design). The undulator curve is actually an envelope; the detailed spectral dependence is shown in Figure 2. Right: The approximate relationship between the electron-beam oscillations for the bending magnet (bottom), wiggler (middle), and undulator (top), and the respective angular distributions of their radiation. Undulator radiation is emitted in an intense laser-like beam.

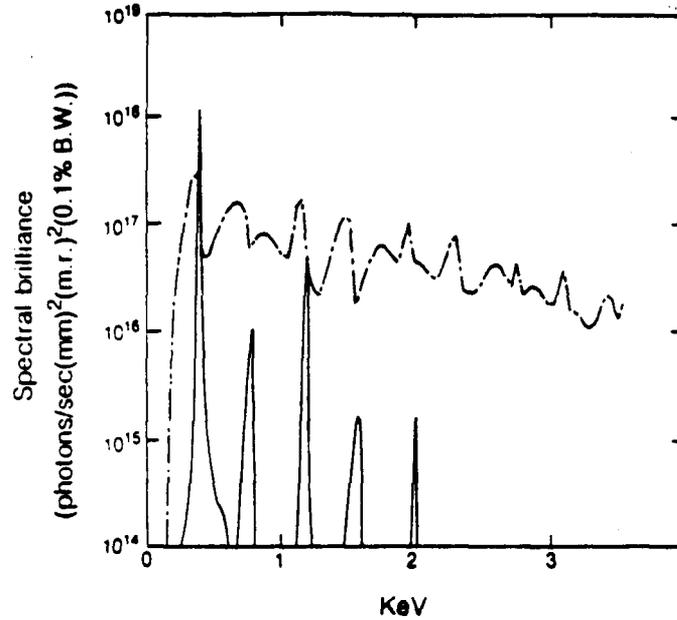


Figure 2. Spectral Brilliance as a Function of Photon Energy. Spectral brilliance through a pinhole aperture as a function of photon energy is shown for the 400-eV-fundamental-energy undulators of Table 1, for both the 1.3-GeV ring (solid line) and the 6-GeV ring (dashed line). The spectral brilliance and purity of the 1.3-GeV machine is diminished at 6 GeV, while the power to the optical element is increased.

Footnotes: Insertion-Device Properties

The fundamental wavelength λ_p of an undulator of period λ_u at an opening angle σ is:

$$\lambda_p^m = \frac{\lambda_u}{2\gamma^2 m} \left(1 + K^2/2 + \gamma^2 \sigma^2 \right) \quad (\text{FN1})$$

The radiation is emitted into an opening angle

$$\Omega = \left(1 + \frac{K^2}{2} \right) \frac{1}{N\gamma^2} = \frac{2\lambda_p}{L} \quad (\text{FN2})$$

The power in the fundamental is:

$$P(\lambda_p) \propto \frac{K^2 N}{1 + K^2/2} \quad (\text{FN3})$$

The ratio of the total power to the power in the fundamental is:

$$\sum_m \frac{P_m}{P_1} = 1 + K^2/2 \quad (\text{FN4})$$

The total power from the device is:

$$P_T = 0.127 (E(\text{GeV}))^2 \langle B(\text{kG}) \rangle^2 L(\text{cm}) I(\text{A}) \quad (\text{FN5})$$

Table 1

Undulator Performance on 1.3- and 6-GeV Machines

Conditions: The total power is constant in the comparison between the 1.3- and the 6-GeV rings at any energy, assuming that $E^2 B^2 L$ is constant. That is, the beam current is fixed (at 400 mA) in the comparison.

Machine Energy (GeV)	E_1 (eV)	λ_u (cm)	B_0 (T)	K	N	Total Power (W)	Power Density at 10 m (W/mm^2)	Power in the Central Spot (W)	Brilliance (photons/s $\cdot mm^2 \cdot mrad^2 \cdot 0.1\% BW$)
1.3	100	10	0.12	1.1	50	30	0.7	1.6	3.2×10^{17}
6	100	95.5	0.0255	2.27	5	30	7	16	4.9×10^{16}
1.3	200	5	0.236	1.1	100	120	3.0	4.5	1.3×10^{18}
6	200	47.7	0.051	2.27	10	120	29	43.5	1.9×10^{17}
1.3	400	3.5	0.165	0.54	142	58	3.00	3	1.2×10^{18}
6	400	42.5	0.035	1.42	12	60	24	24	3.1×10^{17}
6	15,000	2.15	0.176	0.355	230	1400	1700	850	4×10^{18}

Undulator Performance and Storage-Ring Design:
The Need for Two Machines

Footnote 1 provides the basis for choosing the energy E of the machine necessary to produce a $K = 1$ device operating in the range $0.5 \text{ \AA} < \lambda_p < 1.0 \text{ \AA}$. For a fixed-length straight section, it is best to make the period λ_u as small as possible for $K = 1$. The limit on λ_u is determined by magnet technology and results in a machine-energy requirement of 6 GeV. There is a similar optimum energy of about 1.5 GeV for producing fundamental undulator radiation with $\lambda_p > 10 \text{ \AA}$. Nevertheless, there is a basic asymmetry between the two machines: A high-energy machine can produce lower-energy undulator radiation by making λ_u or K larger, but a low-energy machine cannot produce first-harmonic radiation in the x-ray region because of the lower limit on λ_u . To use higher harmonics for this purpose requires large K and greatly diminished brilliance. Let us consider in more detail two important technical issues relevant to our recommendations: (1) the problems of producing soft x-ray ultraviolet (XUV) ($\lambda_p < 10 \text{ \AA}$) undulator radiation on a 6-GeV machine and (2) the thermal loads generated by hard-x-ray undulators on a 6-GeV machine.

(1) To produce $\lambda_p = 10 \text{ \AA}$ with $E = 6 \text{ GeV}$ requires a reduction in N (an increase in λ_u , for fixed L) and changes in either K or B or both. Table 1 compares XUV devices on the ALS machine with devices to produce the same λ_p on a 6-GeV machine. In this comparison K and B are changed in the device in such a way as to keep constant the total power produced. The result for the 400-eV device, for example, is a reduction in brilliance on the 6-GeV machine by a factor of four and a concomitant increase in the power in the central spot by a factor of eight. Clearly, the beam quality has diminished. Also, the power densities may exceed those tolerable on delicate XUV monochromators. In addition, the spectral purity is decreased, as shown in Figure 2.

(2) The power densities produced by hard x-ray undulators are clearly high, as demonstrated by the last entry on Table 1. This issue will be the subject of substantial research and development during the preparation of proposals for 6-GeV facilities. It is, however, already clear that the total power and power density can be withstood by properly engineered nonoptical components. This conclusion follows from considering the powers and power densities created in fixed-target x-ray tubes ($\sim 1/2 \text{ kW/mm}^2$). Starting from the power density of 2300 W/mm^2 at 10 meters that is listed in Table 1, adjustments should be made for the placement of components at larger distances from the source and for the implementation of oblique-incidence geometries. Furthermore, for purposes of the comparison in Table 1, the same currents were used for both machines. It is unlikely that a 6-GeV machine would have such a high current. The combination of all these factors diminishes the expected power densities to a few tens of W/mm^2 , well below known thermal limits for nonoptical components. Further research and development will be necessary to develop thermally robust optical components, but the situation is clearly less critical than for XUV optics.

To use a 6-GeV ring for soft-x-ray science, the higher-order power from the beam must be removed before the beam strikes the first focusing optical element. There exists in principle a solution to the higher-order-power problem, using

total-external-reflection optics. The basic concept is that by properly choosing the mirror material and the angle of reflection, the unwanted high-energy photons can be absorbed on the first metal mirror. This is common practice in the hard x-ray region. For the XUV region, an aluminum mirror at 30-mrad incident angle would absorb the higher harmonics well at energies between 800 and 1000 eV. A fundamental difference between work in the XUV and the x-ray regions is that experiments in the XUV commonly span up to two decades in energy (e.g., 20 eV to 2000 eV), while in the x-ray they rarely span a factor of two. Utilizing the total-external-reflection phenomenon in the XUV region is thus much more complicated because for every factor-of-two energy range, a separate mirror is needed. Use of the total-external-reflection phenomenon in the XUV will be further complicated by carbon contamination of the mirror, which is more of a problem in the XUV and which occurs at a higher rate on a 6-GeV ring. Research and development will be needed to determine the extent to which utilizing the total-external-reflection phenomenon can make a high-energy ring useful in the XUV region. While the above problems can be extreme on a new 6-GeV ring, they are much reduced on a 2.5-GeV machine like the NSLS.

In addition to the power-handling problem, the time structure of a 6-GeV machine will be worse than that of an ideally designed small ring by a factor of two to five. In principle, short pulses could be attained with a 6-GeV ring; this is accomplished with lattice changes and optics and rf-driver modifications that are more complex and expensive on a 6-GeV ring than on a 1.3-GeV ring. The cost of UV beamlines will also be higher on a 6-GeV ring, due to the scaling in size and the more complex optics.

Conclusions

Given these considerations, the need for separate machines optimized in the hard and soft x-ray regions, respectively, becomes apparent. In determining the relative priority of the two machines, there are two factors to be considered.

1. There are no dedicated facilities where hard x-ray undulators can be developed, whereas some limited opportunities for developing XUV undulators do exist.

Of the two high-energy ($E > 4$ GeV) storage rings operating in the USA (PEP and CESR), neither has any prospect of dedicated operation. Nevertheless, important experience could be gained by developing undulators for research-and-development purposes on these rings. Such a device is now part of the SSRL (Stanford Synchrotron Radiation Laboratory) Enhanced Photon Flux Facility (SEPF) construction project.

On existing dedicated lower-energy rings (the SPEAR, Aladdin, and NSLS rings), undulators to serve the XUV regime are now under design or construction. Because other undeveloped straight sections exist at these facilities, new construction could be undertaken to further increase the XUV capacity.

2. Although the low-energy ring cannot provide undulator capability in the x-ray region, the high-energy machine can access some of the XUV region, albeit with reduced performance.

The production of x-rays on a low-energy ring is limited to the use of high-field wigglers. Although these sources do not represent an improvement in flux over beams produced by bending magnets on SPEAR and at NSLS, they would represent an increase in capacity.

Soft x-ray undulator radiation produced on a high-energy machine would have a brilliance that is lower than that produced on an optimal lower-energy machine but higher than that produced by existing devices. Therefore, in principle, the high-energy machine could provide new XUV capability. However, two substantial difficulties arise. First, the spectral purity is compromised, and second, the power in the central spot may exceed the power-handling limits of current optical technology.

SCIENCE AND TECHNOLOGY

Introduction

The properties of insertion devices as sources of radiation are clearly impressive, yet our recommendations must ultimately have a scientific foundation. In our deliberations, the scientific case presented in this section gradually emerged. While not exhaustive, the range of topics presented here does reflect the cross-disciplinary breadth of synchrotron radiation (SR) research.

This section presents brief descriptions of individual research topics, descriptions that are divided into the general areas of techniques and applications. The bulk-structure, surface-structure, and electronic-properties sections discuss general capabilities, accomplishments, and future opportunities offered by enhanced brilliance. Sections on imaging techniques and emerging techniques discuss substantially new approaches made possible by new capability. The applications sections present more specific examples of the types of fundamental and technological problems to which SR can be applied. These examples show that while SR research has a strong fundamental character, it also has a growing relevance to technology.

Experimental Opportunities for Science and Technology

Bulk Structure

X-ray-Absorption Spectroscopy (EXAFS and NEXAFS) -- The extended x-ray-absorption fine structure (EXAFS) technique is among the most widely used and mature of SR methods for determining local structure, and it is the method of choice for structural investigations in certain disciplines. Important results have been obtained in the fields of catalysis, biology, metallurgy and materials science, and surface science, to name just a few.

EXAFS specifically deals with fine structure at $E > 50$ eV above an absorption threshold. In addition, analysis of near-edge x-ray-absorption fine structure (NEXAFS)--also referred to as XANES (x-ray-absorption near-edge structure)--for $E < 50$ eV above an absorption threshold, can provide comple-

mentary information on local electronic and atomic structure and has found equally broad applications.

EXAFS and NEXAFS are discussed in detail in the following sections that deal with the different individual areas of study in which they have been applied. Particularly important examples of the application of these techniques are found in the sections on biology, metallurgy, micromineralogy, catalysis, and surface structure. An example of their application to biology is the determination of the structure of the active site for nitrogen fixation in nitrogenase. The structure of nitrogenase is illustrated in Figure 3.

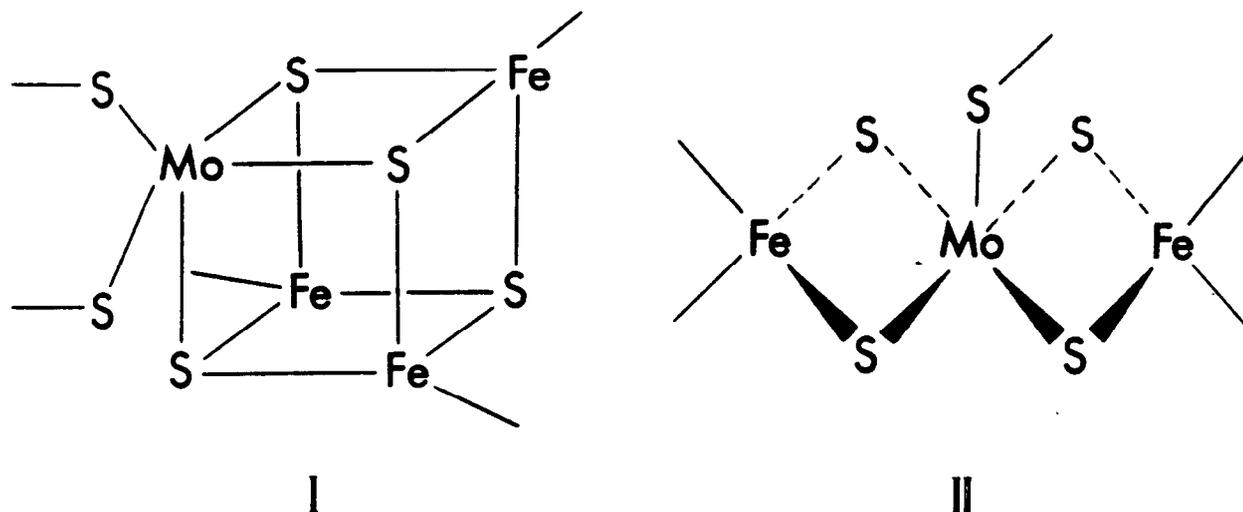


Figure 3. The Structure of Nitrogenase. The enzyme nitrogenase is responsible for the conversion of atmospheric dinitrogen into ammonia, which can be assimilated by growing plants. The structural aspects of the molybdenum site in nitrogenase, where this conversion reaction is carried out, were elucidated for the first time by EXAFS, thus stimulating activity toward synthesis of inorganic analogues.

Bulk Crystallography -- Crystallographic research carried out in the past few years at synchrotron x-ray sources has led to significant advances in a number of areas, notably including the study of anomalous dispersion and of diffraction from very small single-crystal samples. In addition to measuring large anomalous-scattering effects near absorption edges and demonstrating the enormous power of methods of crystal-structure determination utilizing the tunability of synchrotron sources, recent studies are uncovering fascinating dichroic effects associated with "white line" resonant absorptions. X-ray-diffraction data have now been obtained from crystals less than 20 μm in diameter, thus opening up the possibility of structural analysis of a wide variety of technologically-important substances such as zeolite molecular sieves. Areas of crystallographic research with SR that are still largely unexplored but that offer great promise include the determination of electron-density distributions in solids (using ultra-high-resolution diffraction data) and the study of time-dependent structural effects, e.g., the response of materials to pertur-

bations such as laser excitations or varying electric fields. These time-resolved applications will require advanced high-speed parallel data-collection systems with position-sensitive detectors.

Some very significant advances may be expected in many areas of powder diffraction because of the improved resolution available with SR. For example, it will be possible to apply the Rietveld technique, which involves fitting the complete diffraction profile to some structural model, to the analysis of considerably more complex structures having perhaps as many as 100 to 200 parameters and also to the study of phase transitions in which there is a very small distortion of the structure. Other important applications of SR are to peak-shape analysis for particle size, strain broadening, disorder, and thermal diffuse-scattering effects; to search-and-match techniques; and to the indexing of unknowns. Anomalous-scattering methods will be very useful in powder studies, in order to contrast specific elements, especially when they are present in low concentrations in multiphase systems such as supported catalysts.

Surface Structure

A crucial problem in the study of solid surfaces is the determination of atomic positions or bonding geometries for species within the first few atomic layers. Atomic-structure information is essential to understanding the basic physics responsible for the surface structure and the properties of that surface (such as chemical reactivity). Historically, the most useful surface-structure information has come from the "surface sensitive" probes: electrons, ions, and neutral atoms. However, with the advent of SR, the photon has emerged as the most versatile of probes. Photon-based surface-structure techniques can be surface sensitive under some circumstances and highly penetrating under others. In the case of x-ray diffraction, crystallography techniques, which have routinely yielded the atomic structures of most known bulk crystals, are now being used to determine surface structures. When local-structure information is desired, spectroscopy techniques such as surface extended x-ray-absorption fine structure (SEXAFS), NEXAFS, and photoelectron diffraction have been applied with great success. The following sections discuss each of these techniques in more detail.

SEXAFS -- The SEXAFS technique applies the concepts of the established (bulk) EXAFS technique to the determination of atomic arrangements at surfaces. Like EXAFS, the SEXAFS technique measures the x-ray absorption coefficient of an atom that is selected by its absorption edge. The detailed modulations of the x-ray-absorption coefficient, which are caused by the scattering and interference phenomena of the excited photoelectron wave, are used to probe the local environment of a selected atomic species in the surface complex. Measurement of the x-ray-absorption coefficient is accomplished in a surface-sensitive mode, usually by means of total-electron-yield or Auger-electron-yield detection. Fourier transformation of the measured modulations yields very accurate (± 0.01 Å) measurements of the lengths of the bonds between the selected surface atom and its neighbors, as well as its coordination number. These positional accuracies are 5 times higher than those of the electron-diffraction methods that were previously used and developed. The power of SEXAFS lies not only in its accuracy but also in its applicability to disordered surface complexes whose local structure could not previously be resolved.

Since the beginning of SEXAFS spectroscopy in 1978, the technique has been developed into a reliable surface-structure tool. About 30 surface-structure determinations have been successfully carried out so far, including the determination of the structure of atoms and molecules bound to metal and semiconductor surfaces and the determination of the growth of metal/semiconductor interfaces. The technique now has a sensitivity of about 1/3 of an atomic surface layer. Next-generation x-ray and soft x-ray sources will permit sensitivity increases of 100 to 1000 times and will make it possible to carry out experiments much more rapidly, in order to observe time-dependent dynamic effects. With increased brightness of the x-ray source, it will also be possible to develop a microscope based on SEXAFS than can be used to study the structure of surface regions approximately 1 μm in size.

NEXAFS -- A technique related to SEXAFS is NEXAFS, also referred to as XANES. NEXAFS involves the modulations of the x-ray-absorption coefficient within about 50 eV of the excitation threshold. This energy region, which is usually ignored in the SEXAFS analysis, provides important structural information that in many cases is complementary to the information obtained through SEXAFS. It is this region that exhibits the largest modulations of the absorption coefficient and that is therefore the most easily recorded experimentally. The theoretical interpretation of the near-edge structures was first tested on gas-phase molecules and recently has been applied to chemisorbed species, like hydrocarbons on transition-metal surfaces. NEXAFS makes it possible to use a technique that is sensitive to molecular structure to monitor chemical-reaction processes of molecules on surfaces. NEXAFS readily reveals the molecular orientation, the hybridization of the intramolecular bonds and the intramolecular-bond lengths. The importance of such information lies in the elucidation of the catalytic-reaction paths of molecules on surfaces. The sensitivity of NEXAFS is now about 1/10 of an atomic surface layer. Again, improved x-ray sources will greatly increase the sensitivity. More importantly, because of the large size of the modulations and the relatively small energy range (50 eV) needed for NEXAFS studies, it appears that it will be possible to record a complete NEXAFS spectrum in a short time interval and thus record time-dependent phenomena.

Surface Crystallography -- Developments in this field demonstrate the potential for making surface-structure determination as routine as conventional crystallography. The variety of systems amenable to study is large because the high synchrotron flux provides reasonable signals even from low-Z materials and because the penetration depth allows studies of deep layers and interfaces. Contrast with the substrate or the bulk can be achieved naturally (if the adsorbate or reconstructed structure is incommensurate), by employing anomalous scattering techniques with the adsorbate atom of interest, or by using an adsorbate to "decorate" a reconstructed surface. The penetration depth can be varied from the bulk absorption length in normal incidence to the extinction length in a total-external-reflection geometry.

Surface reconstruction is one of the most interesting of surface-structure problems. So far, experimental work has been carried out on the reconstruction of the (100) surface of germanium, and plans are underway for studies of the 7 x 7 structure of silicon. Preliminary studies of the Au(110) surface have demonstrated that in very favorable cases, high-intensity rotating-anode x-ray sources provide enough flux. However, it is clear that the wider possibilities using synchrotron sources will eventually include much more ambitious structural

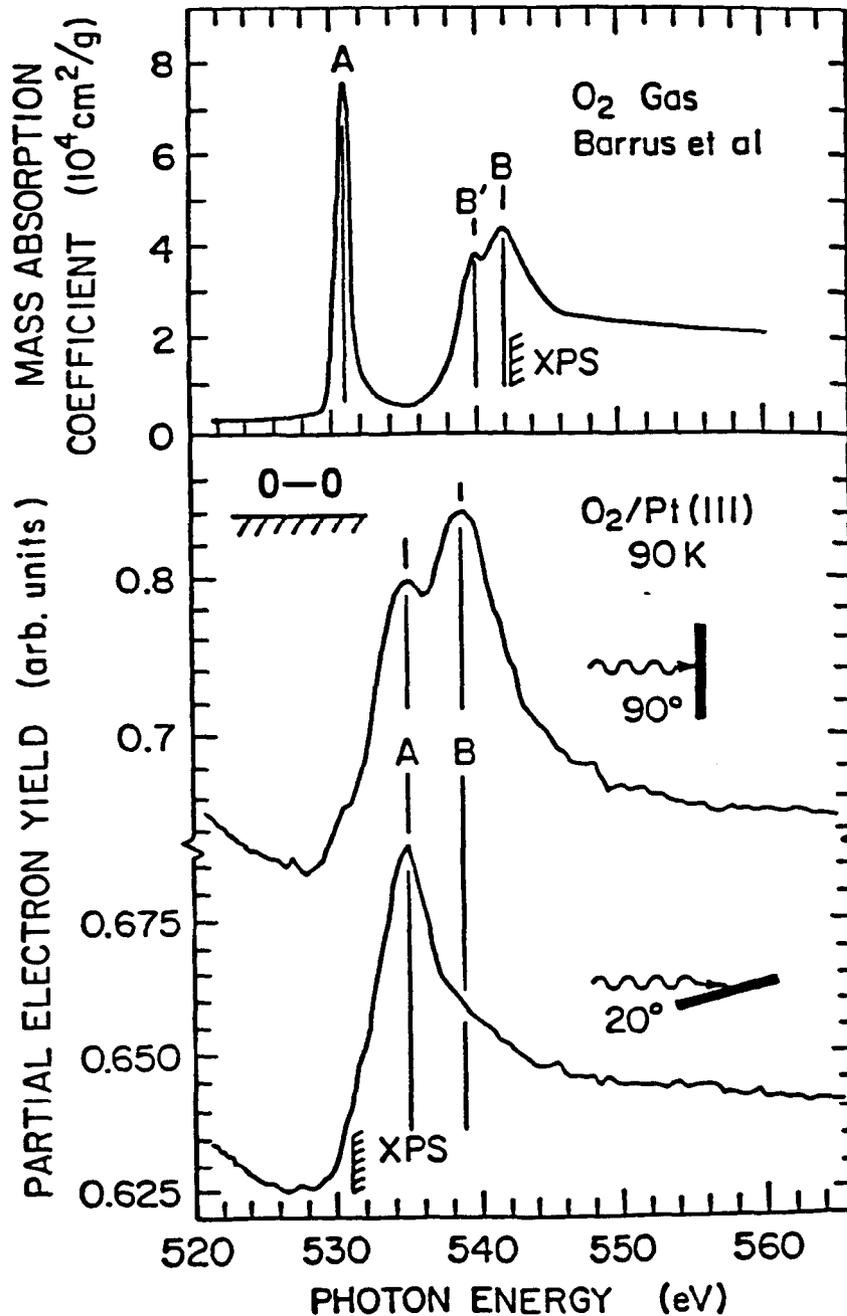


Figure 4. An Application of NEXAFS. This figure provides an example of the use of the NEXAFS technique to determine the orientation of an adsorbed molecular species, O₂ on Pt, utilizing the sensitivity of the π and σ resonances (A and B, respectively) to the polarization of the photon beam. The measurement determined not only that the oxygen was molecular on the surface, but it also determined the orientation of the oxygen and the O-O bond length.

work involving more complex systems and smaller atomic motions. In the latter category is work on the reconstructed surfaces of transition metals such as tungsten and molybdenum. Another category of reconstructed surfaces involves insulators, about which very little is known because they cannot be studied with electron techniques.

Adsorbate systems have received substantial attention so far, perhaps because the surface preparation involved is often simpler than for reconstructed surfaces. Studies of lead monolayers on single-crystal copper have revealed a metastable commensurate structure and a stable one-dimensional incommensurate structure and have documented the melting process at high temperatures. A variety of experimental studies of adsorbates (Xe, Kr, O₂, CF₄, Ar, N₂) on various graphite substrates, including single crystals, have been conducted. Important issues include incommensurability, orientational epitaxy, and the nature of various phase transitions (see the later section, "Phase-Transition Physics").

A number of studies of thin films have been carried out in two principal categories, amorphous films (studied by anomalous scattering) and freely suspended liquid-crystal films. This work has revealed a number of exciting physics and materials-science issues and promises to be a very active area as synchrotron beamlines become more generally available. X-ray beams that are more intense and more highly collimated would make possible a host of improvements in these studies: (1) extension to a wider variety of systems, (2) increased resolution, (3) the development of diffraction microscopy, and (4) time dependent studies, such as was pioneered recently in work on Si and Ge recrystallization following laser annealing.

Photoelectron Diffraction -- In this technique, as in SEXAFS/NEXAFS, core-level excitations are involved, but the emitted-photoelectron intensity is measured in a specific direction. Diffraction associated with photoelectron scattering from various atoms near the emitter produces modulations in intensity as a function of either the emission direction or the incident-photon energy. Changing the photon energy changes the diffraction by altering the electron wavelength, as in SEXAFS.

Such measurements are found to be very sensitive to the type of surface bonding site involved and have also been shown to be capable of determining adsorbate positions to within approximately 0.05 to 0.01 Å. Although such measurements have been carried out over photoelectron energies from approximately 30 to 1500 eV, working at energies greater than 200 eV results in a single-scattering process similar to that used in SEXAFS. Applying Fourier-transform methods to data obtained by scanning the photon energy may yield bond distances very directly. In addition, at energies greater than 1000 eV, simple forward-scattering from nearest-neighbor atoms can produce peaks in intensity along bond directions, thus providing very direct structural information.

Systems studied so far have included atomic and molecular adsorbates on metals and semiconductors, metal/semiconductor interfaces, and layered compounds. Adsorption on stepped surfaces used as models for catalysts has also been studied. Thus, a wide range of problems is accessible with this technique.

In studies of very dilute surface species, the high intensity and tunability of SR is crucial for future work. However, the lack of SR sources in the

difficult region of 500 to 1500 eV has led to a considerable number of high-energy studies being performed with standard x-ray sources. Using these sources, angle scans may take several hours, so it is clear that next-generation SR sources planned for this energy regime will much facilitate photoelectron diffraction. In addition, the directional selectivity required in the diffraction measurement reduces intensities by a factor of approximately 100 below those in SEXAFS, so that higher-intensity sources are needed over the full spectral range from 100 to 1500 eV. Having a much-higher energy resolution of approximately 0.1 eV would also permit separate study of the diffraction effects associated with different chemically-shifted core peaks; for example, diffraction from first-layer and second-layer atoms could be distinguished for certain surfaces. Finally, a very finely focused photon beam should permit such measurements with a spatial resolution of 20 μm or less.

Electronic Properties: Bonding Structure and Dynamics

Photoemission from Solids and Solid Surfaces — Photoemission refers to the measurement of the energy distribution of electrons emitted when a photon is absorbed by matter of any form. Photoelectron spectroscopy has always been a very useful tool for probing the electronic states of atoms, molecules, and solids, but the use of SR sources in the last 10 years has revolutionized this field.

1. Angle-Resolved Photoemission

Angle-resolved photoemission has become to electronic structure what x-ray scattering is to crystallography and neutron scattering is to phonon structure. In general, given a single crystal, the three-dimensional bulk or the two-dimensional surface band structure can be determined. The unique capabilities that are available with a polarized, tunable, and intense radiation source allow the experimenter to tune to any part of the two- or three-dimensional band structure and to determine the orbital symmetry of each state. These simple symmetry rules have been used to determine bulk band symmetries, surface state (intrinsic or extrinsic) orbital character, and the bonding orientation of adsorbed molecules. Electronic-structure measurements have been made on such materials as simple metals or semiconductors, transition metals and rare-earths, compound semiconductors and alloys, and intercalated graphite and layered compounds.

Angle-resolved-photoemission measurements on surfaces of single crystals have revealed in detail the character of the two-dimensional states for clean surfaces, i.e., surfaces with atoms or molecules adsorbed from the gas phase or with bulk impurities segregated to the surface. Not only can the electronic states of the adsorbate/substrate bond be observed, but the adsorbate/adsorbate interaction can also be measured, either directly or through the substrate.

2. Core-Level Spectroscopy

There is a type of photoelectron spectroscopy that is conceptually different from the type described above; it involves removing electrons from core levels instead of from the valence or conduction bands. This type of experiment, which is called ESCA (electron spectroscopy for chemical analysis), measures the binding energy of core levels as a function of the bonding configuration

of the atom. The binding energy depends upon the surroundings of the atom being studied, such as the coordination number and the charge transfer. For example, the 4f core level of Ta will shift approximately 0.4 eV for a surface atom compared to the bulk atom, and adsorption of oxygen will cause a chemical shift of approximately 1 to 2 eV. The inherent line width of these 4f states is approximately 0.1 to 0.3 eV.

The advantages of SR for these core-level studies lie in the energy resolution, tunability, and intensity. A resolution of 0.1 eV is available from up-to-date grating monochromators. The tunability of the synchrotron makes it possible to either optimize the cross section or to select a kinetic-energy regime to accentuate the bulk or surface contribution to the spectra. This form of high-resolution ESCA has been used successfully to observe such phenomena as the various oxide states of a surface such as Si; the difference in surface chemistry on terrace or step sites; the shift in core levels at the clean surface compared to that in the bulk; the shift induced by chemisorption of a foreign atom or molecule; and the charge transfer in intercalated graphite.

An example will clearly demonstrate the impact of synchrotron core-level spectroscopy. On a Pt(111) crystal there is a 0.32-eV reduction in the $4f^{7/2}$ binding energy of a surface atom compared to that of a bulk atom, but a Pt atom at a step edge on the surface experiences a 0.58-eV reduction in binding energy. Once the step atoms were identified, the experiments showed that CO adsorbed onto a surface with steps bound preferentially to the Pt atoms at a step, thus causing the binding energy of the Pt atom to increase by 1.29 eV (0.7 eV higher than the binding energy of a bulk atom). This observation was expected, due to charge transfer from the Pt d-states into the CO 2π level during the process of bonding. In contrast, this study showed clearly that the addition of K as a catalytic promoter did not donate electrons to the Pt d-states as all models had predicted, thus suggesting that the simple models for alkali promoters must be reevaluated.

3. The Future with Insertion-Device Machines

For most problems, angle-resolved photoemission can be accomplished with the intensity and resolution available with the current-generation bending-magnet machines. However, there are several modifications of the conventional experiment that require considerably more brightness. In contrast to angle-resolved photoemission, high-resolution core-level spectroscopy can benefit immensely from the new-generation insertion-device machine.

The ultimate angle-resolved-photoemission experiment should resolve not only the energy and momentum of the emitted electron but also the spin polarization. The limitation is the 10^{-3} to 10^{-6} efficiency of spin-polarization detectors. Given the capability to resolve spin polarization, the detailed character of the exchange splitting and the spin polarization as a function of temperature could be determined for any point in the two- or three-dimensional band structure; phase transitions in rare-earth intermetallic compounds could be investigated; current theories of itinerant ferromagnetics could be tested; and magnetic properties of surfaces could be investigated.

A study of magnetic surface properties has recently been carried out in Europe. Figure 5 shows angle-resolved-photoemission spectra from a specific point in the surface Brillouin zone of Ni(110). The two peaks near the Fermi

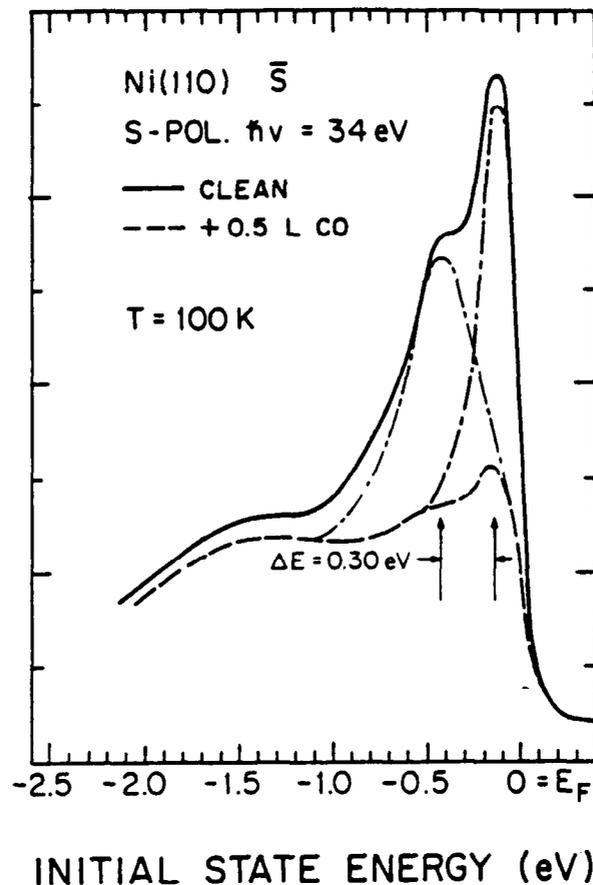


Figure 5. Angle-Resolved-Photoemission Spectra from Ni(110)

energy are surface states, one from the majority spin band and the other from the minority band. The exchange splitting is 0.3 eV, approximately equal to the bulk exchange splitting of Ni. This measurement clearly shows that the surface of Ni is not magnetically "dead." Future work will measure the net macroscopic polarization in each state as a function of crystal temperature. The local exchange splitting will persist above the Curie temperature, but the polarization will disappear. Such an experiment would lead to an understanding of the surface magnetization, including both the surface Curie temperature and the magnetic domain size. Eventually one wants to study the magnetic properties of surfaces that are contaminated with impurities.

Clearly, undulators would make spin-polarized experiments as easy as angle-resolved photoemission is today. It is important to be able to tune the incident polarization; such control could be achieved by means of a combined vertical and horizontal undulator. The momentum resolution of most energy analyzers now used at synchrotron facilities is too large for studies at higher photon energies or for samples with large unit cells. A reduction of an order of magnitude or more in signal will result when the momentum resolution is improved. The new high-brightness insertion devices will allow measurements to be routinely conducted with better energy and angular resolution.

Modern grating monochromators specially adapted to the unique source characteristics of a storage ring promise to give a resolution of better than 0.1 eV (up to 1000 eV). To estimate the flux available at this resolution, it can be noted that a typical commercial ESCA instrument using an Al target at 1 kW delivers approximately 10^{12} photons/s/30 mm². The inherent resolution due to the Al_{Kα} line width is 0.83 eV. When the resolution is improved to approximately 0.3 eV by using any of the commercial 0.5-meter quartz-crystal monochromators, the counting rate is reduced by approximately two orders of magnitude. In contrast, a new toroidal grating monochromator will conservatively yield 4.0×10^{10} photons/s/mm² at 0.3 eV resolution when coupled to a bending magnetic with a 0.5-A beam current. This performance is an improvement over that available with commercial ESCA instruments, but it is probably not significant enough to bring a large majority of conventional ESCA users out of their laboratories.

The performance is considerably better using an undulator on a machine operating at approximately 1 GeV. A good monochromator could produce in excess of 10^{12} photons/s/mm² with a resolution of 0.1 eV. Compared to what is available with conventional ESCA instruments, this performance represents an increase in flux of at least two orders of magnitude and an order-of-magnitude improvement in resolution. Such a capability would allow the study of very small concentrations and dynamical processes. For example, it is quite possible that the thermal evolution of any species such as an adsorbate, impurity, or intercalant could be followed directly.

4. Excitation Experiments

The order-of-magnitude increase in brightness available from undulators will make it quite feasible to measure the angle-resolved-photoemission spectra of normally unoccupied states that have been populated by laser excitation. The few experiments that have been attempted in this area indicate that excitation is accompanied by quite dramatic charge redistribution in the occupied bands.

There are many coincidence-type experiments that become possible with the increased signal available from an insertion device. In many of these experiments, one of the channels is the energy-resolved electron that is emitted either by the direct ionization or by the subsequent Auger decay. The sections in this report on gas-phase spectroscopy and photon-stimulated desorption discuss experiments in which one of the coincidence channels is the ion fragment and the other is the emitted electron. There is also a class of experiments that is concerned with electron/electron coincidence between the primary emission and the subsequent Auger decay. For example, one channel could be set on the surface core-level peak for a step-edge atom, and the other channel could sweep through the Auger signal. This technique would give direct information about the local density of states on an atom located at a step.

Gas-Phase Spectroscopy

1. Current Studies

Gas-phase spectroscopy as practiced at SR facilities is primarily the study of highly excited states of atoms and molecules. This study includes the characterization of the electronic states of these many-particle systems, of the decay channels of the excited states, and of the interaction of the excited

atoms or molecules with other gas-phase molecules. In the last decade, the scientific progress in this small but active area of research has been substantial, and the new generation of insertion devices will lead to revolutionary improvements.

Experimental investigations of the resonance states (shape resonances) in the continuum of molecules, coupled with theoretical calculations, have led to a clear understanding of the origin of shape resonances. The symmetry properties of these resonances are now commonly used to determine the bonding orientation of molecules adsorbed on surfaces, and the energy position of the resonance reveals the bond length of the molecule on the surface.

Experiments in Europe and the USA on the photoionization characteristics of metal vapors are producing a clear picture of the photoexcitation process in transition and rare-earth metals. When the next-generation light sources become available, it will be possible to study multimetal clusters with and without ligands. These experiments will be seminal in identifying the degree of localization of the chemisorption bond on a surface and could be the key to understanding reactions on a finely dispersed catalyst.

Work is also being conducted on photoinduced fragmentation of molecules and transition-metal complexes; this work will have a direct impact on the understanding and the utilization of photon-stimulated desorption (PSD) from solids. In addition, this type of study suggests the use of tunable soft x-rays to stimulate selected chemical reactions that will selectively break large organic molecules.

A final example of the impact of gas-phase spectroscopy on condensed-matter science is the exciting photochemistry being investigated in Europe. This work uses a tunable synchrotron source to preferentially excite molecular ions to specific vibronic states. The ions are then allowed to interact with a second gas-phase species. This work, along with the work described in the previous paragraph, constitutes just the first sign of a new type of photochemistry.

2. The Impact of New Machines

In the future, the new insertion-device-based machines will have a great impact on gas-phase spectroscopy. The signal in most gas-phase-spectroscopy experiments is very low and will benefit spectacularly from the orders-of-magnitude increase in brightness that is offered by these insertion devices. In a gas-phase experiment, the sample density is approximately 10^{-10} times the sample density in an experiment involving a solid, and the required resolution is at least an order of magnitude smaller. For example, in many gas-phase experiments the output signal may be proportional to the machine brightness to the third power, so a 10^4 improvement in brightness would permit qualitatively new experiments. A simple argument will illustrate the dependence of the experiments on brightness.

For a given monochromator design, the output flux per unit energy resolution depends linearly upon the brightness of the source. If the ions or electrons being produced are to be energy analyzed, then the product of source area and accepted solid angle (brightness) is conserved in the analyzer, thus giving another measure that is linearly dependent on the brightness. Also, in many

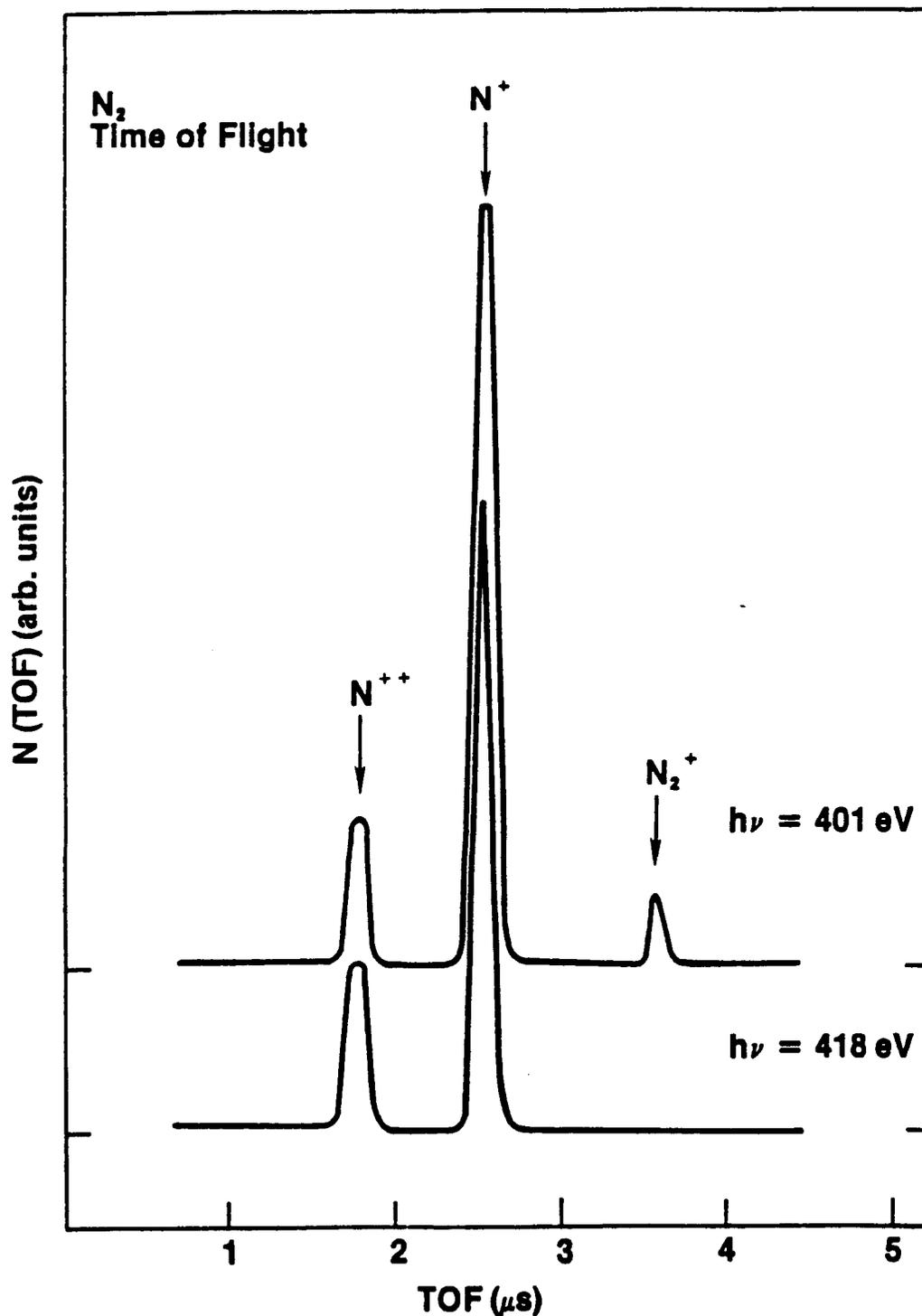


Figure 6. Ion-Fragmentation Patterns for N₂ Near the Nitrogen K Absorption Edge. The singly ionized molecule appears only at 401 eV, the molecular-nitrogen π resonance, where a direct-recombination process results in removal of only a single charge from the molecule. Other Auger decay processes lead to singly and doubly ionized atomic nitrogen.

future experiments, the amount of sample material may be very small, thus requiring small beams and a bright source imaged onto the sample region.

One prototype experiment will clearly illustrate the gains that are possible with the new sources. The core-level ion-fragmentation studies described above were carried out on a bending-magnet beamline. The counting rate for the ions produced was approximately 10 Hz in a peak, and the equivalent counting rate in the energy distribution of emitted electrons was approximately 1 Hz. These rates were accumulated with a photon resolution that was 10 to 50 times poorer than what was needed to fully separate features in the spectra. The experiment that one would like to do requires better resolution in both the incident light and energy analyzer and enough light intensity so that the electron-decay signal and the ion fragmentation can be run in coincidence while simultaneously measuring the kinetic energy of the ions. Such an experiment would require the brightness to be increased by a factor of approximately 10^4 ; it would also require a new monochromator that would produce an energy resolution of 1 part in 10^4 at a photon energy of hundreds of volts.

The new insertion devices will also create the following opportunities in gas-phase spectroscopy:

- A. When a photon excites an atom or molecule, electrons, ions, and photons are emitted as a result of either the excitation process or the resultant decay. An in-depth picture of the dynamics of the process can be obtained by coincidence measurements. For example, coincidence between the energy-resolved electrons and the ion fragments can determine the decay channel. Ion/ion-coincidence measurements will relate the ion pairs in the fragmentation, and electron/electron-coincidence measurements can detect multiple Auger decay or relate structure in the Auger spectra to the initial excitation state.
- B. It will become possible to study the electron energy levels and the lifetime of excited complexes by synchronizing a laser and the short time pulses from the storage ring.
- C. The photoemitted electrons will be intense enough so that they may be run through a spin-polarization detector, which usually has an efficiency of 10^{-3} to 10^{-6} .
- D. The proposal from LBL to couple a vertical and a horizontal undulator to "control" the polarization points the way to a technique that would allow the experimenter to easily investigate the "right" or "left" handedness of complexes.
- E. It will be possible to use dilute supersonic beams or to investigate the interaction in crossed molecular beams.

In summary, these new and bright insertion-device sources will open up new frontiers in gas-phase spectroscopy for exploring in detail the geometric and dynamic properties of atoms and molecules in electronic states previously inaccessible.

Photon-Stimulated Desorption (PSD) -- PSD is a relatively new application of SR that has both promise as an analytical tool and the potential for provid-

ing some new insight into the energetics and dynamics of highly excited surface-bonding states. The analytical usefulness arises from the highly specific nature of the desorption process. Desorption occurs only from the surface layer and only from the surface-bonded complex that is electronically excited by the incident radiation. Thus, surface- and site-specific information can be derived for the desorbed species by analyzing the spectral dependence of the desorption (by means of NEXAFS and EXAFS), as discussed in the preceding sections on surface structure. Surface structure can also be directly analyzed through the study of ion-angular distributions. There are a number of important problems of fundamental and technological interest regarding which desorption can provide unique insight. Two examples of such problems are:

1. Catalysts and Catalyst Supports -- Catalysts in general have complex surface structures whose chemistry is dominated by minority sites. The site and adsorbate specificity of PSD allows the study of such complex surfaces in a direct way.
2. Hydrogen on Surfaces -- Hydrogen/surface chemistry is critical in a range of technologically important processes, including catalysis, corrosion, semiconductor processing, electrochemistry, ceramic processing, and many others. PSD is very sensitive to hydrogen and can not only define its bonding site but also determine the electronic and geometric structure of the site.

Because desorption cross sections are often extremely small and because systems of interest involve submonolayer coverages, PSD is one of the most "photon hungry" of techniques. In addition, many systems and processes of high importance--e.g., catalysis, corrosion, and ceramic powders--involve the study of small particles, requiring the use of a highly focused photon beam.

Desorption is now known to be induced by multiply excited states in which strong correlation effects lead to unique charge dynamics, which in turn can lead to both high-energy deposition on a site and electronic lifetimes of sufficient length for desorption to occur. Investigations of the physics of this effect will require examining systems with a range of desorption cross sections. One of the most potentially informative of experiments involves the measurement of ion/ion- and electron/ion-coincidence events. These studies require high flux, high spatial resolution, and timing capability. Coincidence experiments are not feasible with bending-magnet sources but could become feasible with insertion-device beamlines. An important adjunct to the desorption experiments is the study of photon-stimulated dissociation of large molecules. This research has had a direct impact on our thinking regarding radiation-induced damage and chemistry.

Imaging and Microstructure Fabrication

Soft X-ray Microscopy -- The term "x-ray microscopy" refers to a broad range of techniques that use soft x-rays to obtain morphological information about small objects. Biological and medical applications of microscopy are the most prominent applications, but others are emerging. The scientific value of these techniques derives from limitations in the present approaches to microscopy. Specifically, visible-light microscopy, electron microscopy, and hard x-ray crystallography all provide excellent imaging capability, but

they have various limitations. For example, consider a biological cell that is 1 to 3 μm wide and that contains interesting structures smaller than $1/4 \mu\text{m}$. It cannot be crystallized. It cannot be viewed with visible light and can only be imaged in the electron microscope if it is dehydrated, sectioned, stained with (maybe even replaced by) heavy metal, and placed in a high vacuum. There are many life-science problems that require a more gentle probe to gather morphological information with less damage than would be done in the electron microscope and to allow the sample to remain in its natural, wet, living state in the atmosphere. Imaging with soft x-rays promises all this plus element discrimination using x-ray-absorption edges.

1. General Technical Requirements

It appears that a breakthrough in x-ray imaging will result from advances in the microfabrication methods developed by the semiconductor industry. Zone-plate lenses with a spatial resolution of 600 Å are being fabricated, and values of 100 to 200 Å are expected soon. This development opens the way to a range of soft x-ray imaging methods, provided that a suitable source is available. This source must have optimum output in the 20 to 50-Å region (covering the O, C, and N K edges), and for imaging it must provide the highest possible coherent power. (This quantity is closely related to the spectral brilliance.) These requirements will be met by an undulator having a large number (e.g., 100 to 300) of periods and operating on a low-emittance storage ring of an energy between 1 and 2 GeV.

For example, the emittance of a spatially coherent, 30-Å x-ray beam is $\epsilon_{30} = 2 \times 10^{-9}$ m.rad. 30-Å photons emitted from a phase-space volume larger than $(\epsilon_{30})^2$ cannot be utilized. As a result 99.99% of the radiation from bending magnets is wasted in imaging experiments conducted on present storage rings; the next-generation storage rings and undulators are very important to this work.

2. Specific Experimental Methods

Table 2 indicates six of the more important methods of x-ray imaging and the improvements expected with the next generation of sources. Only one method (number 1) now gives useful biological results, but most of them will do so given the new sources. The most fully developed methods are numbers 2 and 3, which are already applied to biology. The three-dimensional methods will take longer to develop, but they are of considerably more importance.

3. Specific Examples of Research Problems That can be Approached through Soft X-ray Microscopy

The manner in which bone-matrix vesticles organize themselves and eventually determine the calcium structures that form bone is not well understood. It is expected that this process can be followed using calcium-specific x-ray imaging methods and understood with the help of calcium EXAFS studies, if necessary, on a pixel-by-pixel basis.

Nerve cells can be imaged by conventional means, but there is no easy way to distinguish a joint (a synapse) from a simple overlap. Thus, the "wiring diagram" cannot be understood. With the aid of element-specific x-ray imaging,

Table 2

Six Important Methods of X-ray Imaging

Technique	Promise	Disadvantages	$\frac{\Delta\lambda}{\lambda}$ needs (%)	Status with Present Sources	Next Steps Given New Sources
1. Contact	δ -50A*	2D thin specimens only, damage problems	2	successful biology in progress	3D refinements
2. Zone plate lens imaging	δ -100-200A (zone plate limited)	mainly 2D high damage	0.3	successful trials at δ -600A	achieve δ goal, faster exposures, mitigation of damage problem
3. Scanning through zone plate focus	δ -100-200A (zone plate limited), in- trinsically low damage, integrated with computer	mainly 2D slow speed hence small field	0.3	successful trials at δ -3000A exposures of an hour or so	achieve δ goal, few second exposures, incorporate spectroscopy & microanalysis
4. Scanning reflection systems	δ -few $\times 10^2$ A some 3D capability, high speed	difficult to fabricate	none	trials at δ -3 μ m with high contrast objects	achieve δ goal
5. Holographic microscopy	3D images δ -few $\times 10^2$ A	slow	0.1	trials at δ -1 μ m with high contrast objects	smaller δ shorter exposure with low contrast 3D objects
6. Soft x-ray diffraction	3D images δ -few $\times 10$ A	slow high damage	0.3.	proof of principle stage	reconstructions from single exposure (axial res'n less good)

* δ \equiv resolution

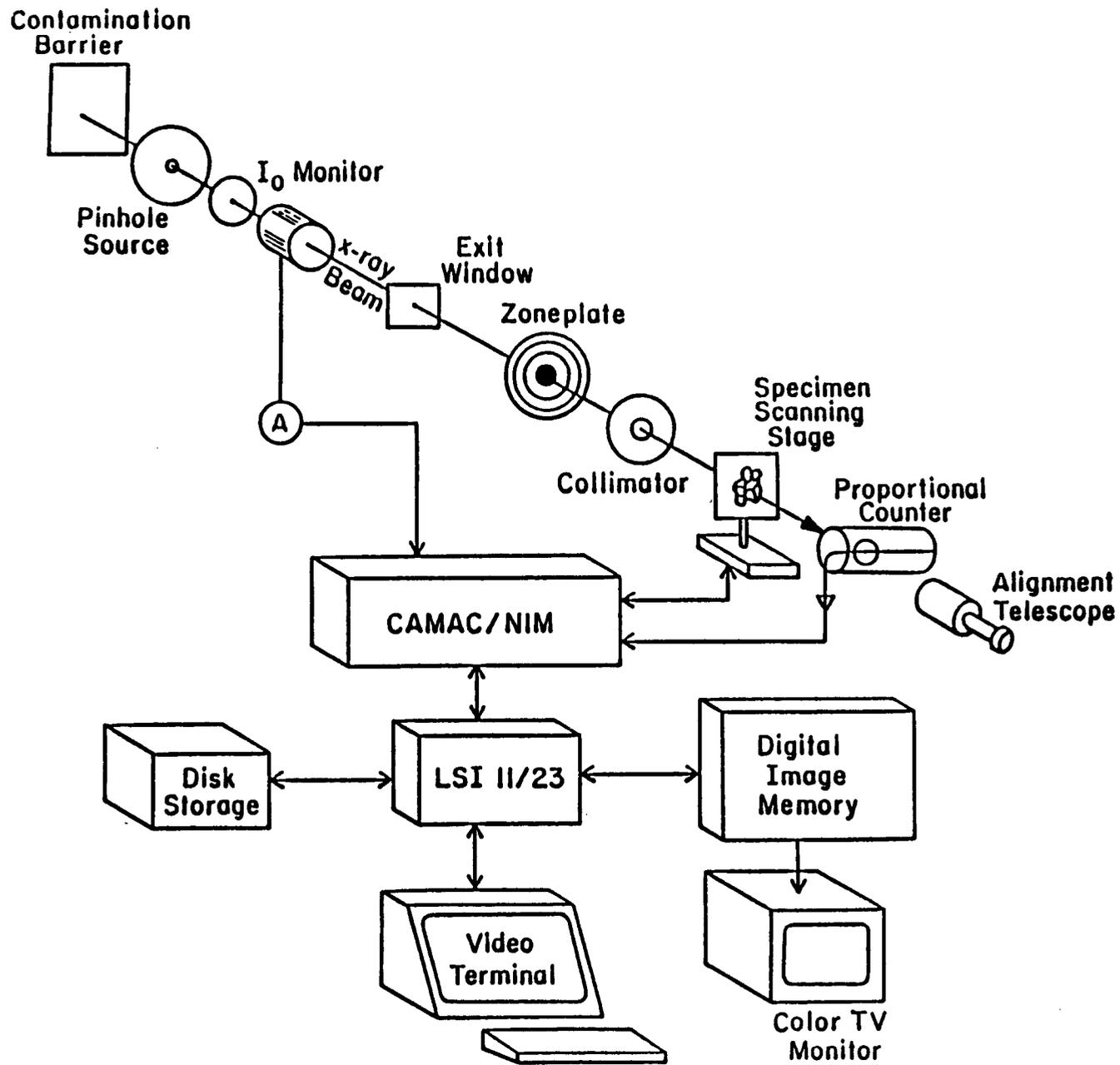


Figure 7. A Soft X-ray Microscope Utilizing a Zone-Plate Lens

SCIENCE AND TECHNOLOGY

it should be possible to highlight the synapses and thus follow the neuron-to-neuron connection sequence.

A similar three-dimensional structural problem is the elucidation of the arrangement of proteins, lipids, carbohydrates and water in ordinary biological cells. This basic problem cannot be solved by ordinary methods even in such well-known cells as blood platelets and bacteria. Bacteria have been chosen for a structural study that uses the C, O, and N K edges to give atomic specificity.

Microprobe Characterization -- Microprobe characterization of materials--an effort that includes both biological and medical applications--involves an investment of over \$500 million nationally in electron microprobe equipment alone. However, x-rays have always been the radiation of choice for microprobe analysis because they provide the following advantages over electron excitation: a 10^3 -better signal-to-noise ratio; cross sections that are higher by a factor of 10 to 10^2 ; reduction by a factor of 10^{-5} to 10^{-6} in the energy dissipated in the sample for the same detectable limit; improved accuracy in quantitative analysis; and the capability for measurements in the presence of air or H_2O (in vivo) with negligible charge collection. Historically, the low brightness of x-ray sources has prevented them from competing with electron sources, both because of the high brightness of the electron sources and because of the ease with which electrostatic and magnetic lenses collect and focus electrons.

With the advent of SR from insertion devices, the performance of an x-ray microprobe can exceed that of a microprobe based on electron sources. To cover the elements of the Periodic Table, an optimal x-ray microprobe requires a tunable undulator insertion device capable of delivering photon energies of from 2 to 33 keV. Obtaining energies of 33 keV from an undulator device requires circulating-electron energies of from 5 to 9 GeV, depending on the intensity of the higher-energy harmonics. Over the energy range of 10 to 33 keV, undulators in such a ring would deliver 10^3 to 10^5 times the intensity produced by current or soon-to-be-completed facilities.

The small angular divergence of the radiation from advanced insertion devices enables x-ray-diffraction techniques using crystals and multilayers to be used for collection and focusing. Thus, the demagnification achievable--just with present technology--would be about 100:1. As a result, spatial resolutions of 500 angstrom-diameters would be achieved in the analysis of bulk samples, as compared with the resolution attainable with an electron microprobe, which is limited by electron spreading in the sample to a level of $1 \mu m^2$. Impurity levels on the order of parts per billion could be detected, compared to the limit of 100 parts per million with an electron microprobe. Diffraction studies of particles smaller than 60 A in diameter would be possible. Auger, photoelectron spectroscopy, and EXAFS analysis could be done in small selected areas of less than $1 \mu m$ -diameter. In summary, the x-ray microprobe would be a highly versatile tool, and many fields of research would benefit from its unparalleled performance.

X-ray Lithography -- The need for an alternative to optical lithography for manufacturing integrated circuits will probably occur in the 1990s, when it will become necessary to achieve a feature resolution of $0.5 \mu m$. Electron-beam systems will be needed to make masks, but they will not be cost effective

for high-volume production in the direct-write mode. Synchrotron x-ray sources thus could become important tools for mass production of integrated circuits.

For microlithography, there are four basic requirements: resolution, registration, throughput, and defect density. Using optical lithography, it is now possible to make lines and spaces that are smaller than $1 \mu\text{m}$ and that are controllable to $0.1 \mu\text{m}$. Optical techniques can be expected to attain a registration error of less than $0.25 \mu\text{m}$ between any two out of eight levels. In order to make x-ray lithography as economically desirable as optical lithography, processing must be done at a rate greater than $1 \text{ cm}^2/\text{s}$. Finally, the defect density must be less than one defect in 10 cm^2 .

Several technological problems must be solved before x-ray lithography can be employed industrially to manufacture electronic devices. The technology for making an x-ray absorbing mask on a thin, x-ray-transparent, dimensionally stable support is probably the most important problem. Another problem involves simultaneously optimizing the source power and the resist sensitivity. Mechanisms for aligning the devices automatically during the exposure must be developed. Finally, a technology is needed for creating large (several square centimeters) high-transmission windows that can withstand the large pressure difference between the evacuated beamline and the lithography chamber.

1. Insertion Devices

The new high-brightness insertion-device synchrotron sources will allow the 4 to 14-A broadband range of the single bending-magnet source to be replaced with a bandwidth of a few percent that is centered at 15 A. Such a move favorably affects the mask-fabrication problem in that the gold-absorber thickness can be reduced from 0.6 to $0.2 \mu\text{m}$, thus allowing $0.2\text{-}\mu\text{m}$ linewidths to be made with 1:1-aspect-ratio masks. Both wiggler and undulator insertion devices are sufficiently powerful and flexible to allow them to be used in an evolutionary way with conventional x-ray-tube technologies or in a revolutionary way at high-contrast, soft x-ray wavelengths (15 A). Wigmblers would likely require a very thin ($1/4$ mil), high-power (10-W) window technology. On the other hand, undulator radiation is sufficiently compact (3 mm) so that differential pumping could be used instead of a window. The undulator also offers an additional degree of scientific sophistication that might ultimately be used to optimize the design of the beam while suppressing power load.

2. Throughput

Conventional x-ray-tube sources have required the development of very sensitive multilayer resist techniques. The throughput of these sources decreases quadratically with linewidth. Synchrotron sources do not suffer from the penumbra problem that underlies that loss and have consequently been pursued for the last several years.

To expose robust single-layer resists, an absorbed dose of 250 to 1000 J/cm^2 is needed in materials like PMMA. At 8 A this dose requirement translates to a flux of 0.25 to $1 \text{ J}/\text{cm}^2$ or 1×10^{15} to 4×10^{15} photons/ cm^2 . Because the x-ray optical-delivery system is only 13 to 17% efficient and because a writing speed of $2 \text{ cm}^2/\text{s}$ is needed to compete with the optical throughput, a source of 1×10^{16} to 5×10^{16} photons/s is needed. This flux requires a 4 to 14-A band-

width for a single bending magnet at 400 mA and has led to a full-spectrum-synchrotron-source approach. The recent development of wiggler and undulator technologies offers the unique possibility of obtaining sufficient power from a very restricted bandwidth. It will be possible to tune the source so as to minimize other technological problems such as mask alignment.

3. Registration and Resolution: Mask Technology

With sources available to date, x-ray masks have required about 0.6 μm of gold absorber. Yet the major application of x-ray lithography will likely be in the 0.5 to 0.2- μm region, due to the success of optical lithography at larger dimensions. A gold absorber with a thickness of 0.6 μm will lead to very high aspect ratios in this region. By shifting to softer x-rays such as 15 A, the mask thickness can be reduced. How far the wavelength can be shifted depends on the window absorption, the mask-substrate absorption, the amount of mask heating, the amount of diffraction, and the resist.

The main limitation involved in going to 15 A is the absorption in the intermediate windows, in the mask support, and in the atmosphere on the way to the resist. Even a 1/4-mil beryllium window produces an almost 3-fold decrease in writing speed, and 1/2-mil windows are unacceptable. Mask heating actually favors the use of 15 A because for a fixed flux level of 100 mW/cm^2 , the incident power on the mask at the exposure rate of the resist is three times higher at 15 A than at 8 A. Diffraction limits the mask to wafer spaces up to 17 μm for 0.2- μm resolution, but this is not a major problem.

Given a 1/4-mil 3-mm x 3-cm window, a high-throughput wiggler lithography system could be built using a neon-gas absorption dip as a filter. However, the energy of the ring may need to be reduced to help eliminate the hard x-ray radiation. For an undulator an opening of 3-mm diameter is sufficient. By using three 100:1-aspect-ratio tubes and differential pumping, a windowless system could be built. Undesired harmonics could be filtered out using neon and helium gas. More sophisticated filtering could be done by using magnesium or multilayer mirrors. Any of these undulator systems would compete with the present optical-system throughput of 2 cm^2/s .

Although either a wiggler or an undulator insertion device might be adequate for x-ray lithography, undulators would offer the prospect of differential pumping, the heat load on the x-ray optics would be much lower, and the power-load-to-output efficiency would likely be higher. Finally, from an engineering point of view, there is an interesting optimum-design problem involved in obtaining the desired beam properties from an undulator magnet.

Emerging Techniques

Inelastic X-ray Scattering -- Dynamic excitations whose energies are on the order of the ambient temperature (so-called thermal energies) play a special role in the physics of condensed-matter systems. Traditionally, excitations in this energy range, below say 100 meV, have been examined using both laser-based Raman and Brillouin techniques for long-wavelength excitations and neutron-scattering techniques, which can cover a larger range of excitation wavelengths. Fundamental limitations in conventional-x-ray-source flux, colli-

mation, and tunability have prevented x-ray techniques from developing the ability to resolve x-ray energy transfers below 1 eV.

The development of synchrotron sources, and particularly the improvements that will be made in the next generation of high-brilliance machines, will make it possible to establish inelastic x-ray-scattering techniques. Studies carried out so far indicate that inelastic scattering with 15-keV x-rays could be resolved at the 1 to 10-meV level, using back-reflection techniques with spherically bent perfect silicon crystals. For better resolution, perhaps to below 1 μ eV, nuclear-resonance scattering from crystals or multilayers made with the Fe^{57} isotope is under active consideration. The only fundamental limit to be discovered so far is the limit imposed by the available source flux per energy bandwidth. For a 1-meV bandwidth, undulator sources on a high-energy storage ring would produce 10^{10} to 10^{11} photons in a beam whose area is less than 1 mm^2 . Such flux levels are considerably higher than those available using neutron sources, so one imagines that a wide range of applications will be possible.

1. Inelastic-Scattering Applications in Condensed-Matter Physics

X-ray techniques will be able to compete in many problem areas traditionally accessed by neutrons, such as the study of phonons between 1 and 100 meV in bulk crystals. However, for certain applications, inelastic x-ray techniques will be unique. These areas include (1) the study of collective electronic excitations to which the neutron does not couple, (2) the range of energy transfers above 200 meV, which is easily accessed with a 15-keV x-ray probe but difficult for the much lower-energy neutron, (3) excitations in disordered materials in which high neutron-energy transfer cannot be produced at small momentum transfer, and (4) the study of systems for which only small samples are available. In the last category, the study of the dynamics of two-dimensional systems should be revolutionized by inelastic x-ray scattering. It should be emphasized that there are, correspondingly, areas in which the neutron probes will remain unique. These include the regime of energy transfer below 1 meV and the study of magnetic excitations.

2. Inelastic X-ray Scattering Applications in Biology

Much of the importance of neutron scattering has derived from its applicability to the study of inelastic processes in solids. Furthermore, neutron scattering is an essential tool for studying hydrogen in biological systems. However, because of the low count rate and large sample size needed, inelastic neutron scattering has found somewhat limited application in biological materials. The development of inelastic x-ray-scattering techniques would have important application to the study of vibrational spectra in biological systems. For example, work on Raman scattering from proteins has suggested that there are anomalous features in the phonon spectrum as a result of a protein molecule being a pseudorandomly folded one-dimensional polymer. This is a kind of "fractal" structure. The understanding of this kind of behavior could help resolve the nature of intramolecular motions in proteins and polynucleotides.

Magnetic X-ray Scattering -- In considering the qualitatively new science that will develop with a high-brilliance source of hard x-rays, the possibility of magnetic x-ray scattering arises. There is a relativistic term in the x-ray-scattering cross section of atoms that is dependent on the magnetization

density. This magnetic scattering is weaker than the conventional Thomson cross section by the square of the ratio of the x-ray energy to the electron mass, which results in a factor of about 1000 for 15-keV x-rays. Further reduction in expected intensity results from (1) the number of magnetic electrons, which is usually small and always less than the total number of electrons, and (2) the form factor of the magnetic electrons, which falls off faster at high momentum transfer than the form factor representing the total charge density. As a result, the magnetic scattering from iron, for example, is weaker than the charge scattering by a factor of 4×10^{-6} . Although the magnetic effect is relatively weak, it should be easily observed with synchrotron sources, and magnetic scattering should mature into an important technique.

Preliminary experiments using conventional x-ray tubes and rotating anodes have succeeded in measuring magnetic Bragg peaks from antiferromagnetic and spin-density-wave materials at intensity levels consistent with the above estimates. On the basis of current experience with conventional charge scattering at synchrotron sources, it is clear that the next generation of high-energy storage rings will enable a variety of magnetic-scattering studies in bulk materials. These studies will have a number of advantages over neutron-scattering studies: (1) small samples (10^{-3} to 1 mm^3) will be quite adequate, (2) the higher resolution (10^{-4} \AA^{-1}) typical of SR will be routine, (3) materials with high neutron absorption (e.g., Cd or Gd) will be easily studied, (4) spin and orbital magnetization effects can be differentiated, and (5) anomalous magnetic-scattering techniques can be exploited. Perhaps more importantly, the intensity estimates are favorable for the study of two-dimensional magnetic structures and the surfaces of magnetic materials. The long-standing problem of surface-enhanced magnetism will be addressed, and it is possible that magnetic-reconstruction effects could be discovered.

Time-Resolved Techniques

1. Picosecond Timing in the Soft X-ray Ultraviolet (XUV)

Response-time measurements in the picosecond range open up a number of interesting possibilities. When a solid or liquid is excited (valence or core electronic excitation), a nonequilibrium-excited-state configuration results, and de-excitation leads to the production of phonons, photons, electrons, and sometimes displaced ions or atoms. Frequently, defects form and atomic rearrangement occurs around the excited atom. Over a period of time of about 10^{-16} second (corresponding to the absorption of radiation) to about 10^{-9} second (corresponding to the final decay processes in the vacuum ultraviolet [VUV]), a host of radiative and nonradiative de-excitations occur that include structural rearrangements. Very little is known about these various channels of decay, especially for core-level excitation.

The potential of a new timing technique, cross-correlation phase fluorometry--employing the short, repeated light pulses from an SR source was recently demonstrated in experiments to measure the luminescence lifetime of a number of organic and inorganic substances. In one case, a fluorescence lifetime of 196 ps was measured with an uncertainty of ± 6 ps. The technique is not constrained to lifetimes longer than the synchrotron-pulse duration. In fact, lifetimes as short as 0.05 ps might be measured with the new high-brightness sources, providing that the pulse structure is stable.

In addition to precise time-structure stability, high brightness is essential in timing experiments for at least two reasons. First, high intensity makes it possible to achieve good signal-to-noise ratios, especially with small samples. Second, highly collimated beams are important to reduce time spread or spatial dispersion in the picosecond regime.

2. Time-Resolved X-ray Scattering

High-resolution x-ray-scattering measurements performed at synchrotrons have yielded considerable insight concerning the equilibrium states of condensed matter. Time-resolved x-ray-scattering experiments will similarly enhance our understanding of nonequilibrium phenomena in liquids and solids. The problems that can profitably be studied using time-resolved techniques come from a variety of disciplines and have many practical implications. Examples are grain-boundary formation and growth in metals, melting, laser annealing, electrical switching, and phase separation in liquids and solid alloys. To date, very few time-resolved x-ray-scattering studies have been carried out. Nonetheless, these few studies have revealed dramatically new information, unavailable from other techniques, on laser annealing in silicon, phase separation in polymers, and switching in ferroelectrics.

The most important attributes that a synchrotron must have to make such studies feasible are high intensity and low emittance. The time structure of the photon flux is not particularly important because the photons are being used as probes of the systems under study. Detection technology borrowed from high-energy physicists will obviate the need to use a pulsed x-ray probe beam to time resolve the scattering data, even in very fast applications. A level of beam intensity that is higher than what is currently available will permit exploration of processes in systems--such as surfaces--with intrinsically small scattering amplitudes and of phenomena that cannot be reproduced at a sufficient rate to permit the use of present x-ray sources for the accumulation of statistically satisfactory data.

Time-Resolution Experiments in Biology

1. EXAFS on a Microsecond to Millisecond Scale

Current studies using energy-dispersive, time-resolved x-ray-absorption spectroscopy have achieved useful EXAFS spectra on a time scale on the order of fractions of a second. The increase in brightness on the order of a factor of 10^2 shows time resolution to be extended down into the submillisecond time scale. It should thus be possible to work on such a time scale in following conformational intermediates in photon-stimulated or chemically stimulated reactions initiated by a photolysis reaction. For example, it might be possible to study the unstable intermediates of the enzyme xanthine oxidase; in this enzyme, intramolecular electron transfer between the Mo site and the Fe/S center is thought to be on the order of or faster than 10 ns.

2. Study of Time-Dependent Phenomena in Biological Membranes

The use of time-synchronized detection in small-angle scattering has been demonstrated in Europe in studies on muscle function that were conducted on a millisecond-to-second time scale. The advent of higher-brightness sources should allow this technique to be extended into the submillisecond time range.

For example, the study of photocycling of bacteriorhodopsin at around 300 μ s would be possible. A photocycle intermediate has been identified in this time scale by observing changes in the UV absorption spectrum after an initiating light flash. Accompanying structural changes could in principle be studied by performing a similar experiment using time-synchronized small-angle x-ray diffraction.

3. Single-Crystal Studies of Atomic Motions in Proteins

With current photon sources it is possible to use two-dimensional electronic detection techniques to collect intensity data for single crystals, on a time scale measured in the range of seconds to minutes. With higher-brightness sources, this time scale might be extended down into the ten-to-one hundred-millisecond time range. It is possible that certain thermally activated conformational changes in proteins, such as the flipover of a tryptophane side group, could be seen on this time scale by studying intensity fluctuations in various Bragg reflections. This kind of "noise spectroscopy" has been used to measure quantities like molecular weights in terms of fluctuations in a dielectric signal. An extension of this kind of fluctuation spectroscopy to x-ray diffraction would provide a new direction in biological-structure determination.

Applications

Metallurgy and Materials Science

Scientists and engineers in the fields of metallurgy and materials science comprise a community that is making increasing use of SR and that will become increasingly involved in developing new applications of this tool as new sources become available. This large community of new users has recognized the utility of synchrotron sources for diffraction, EXAFS, photoelectron-spectroscopy and x-ray-absorption measurements, topography, lithography, small-angle scattering, and fluorescence analysis; but they have not been able to make extensive use of these techniques due to the unavailability of sources (particularly hard x-ray sources). Typical metallurgy and materials-science applications for which the synchrotron sources have unique advantages may be summarized in the following categories.

Diffraction and Scattering -- Structural analysis of small crystals or powders that are not available in the form of single crystals (e.g., zeolites and crystalline polymers) or small precipitated phases can be carried out. In fact, small crystals are often desirable for obtaining accurate electron-density distributions and for minimizing extinction and absorption. Alloy-structure determination for both crystalline and amorphous solids is an important area of future synchrotron research that will utilize the high resolution available in elastic-scattering experiments and the wide wavelength tunability that allows the use of anomalous scattering to selectively probe the structure associated with different elements. These SR capabilities allow studies of alloys comprised of near-neighbor elements in the periodic table.

Structural studies of clustering, precipitation, and spinodal decomposition will also be enhanced by the high brilliance of SR. It will be possible

to study the kinetics of phase changes, including fluctuation phenomena that characterize the early stages of many phase transitions. Studies of the time dependence of crystallization and of the liquid/solid phase change are important areas of investigation for many different types of materials.

The structure of two-dimensional phases such as those at grain boundaries is an ongoing subject of research in which the high brilliance, tunability, and high collimation of synchrotron sources will make important advances possible. For example, the study of metals and ceramics have shown that significant diffracted intensities can be obtained from the small volumes of materials at the grain boundaries.

Finally, the high brightness and tunability of the new sources will allow studies of diffuse scattering in systems that cannot now be adequately studied, such as ternary and quaternary alloys and polymer samples that are comprised of weak x-ray scatterers.

Topography -- Topography in both the white-beam and monochromatic modes will be extensively used to image lattice strains. In this application the methods are complementary to the more commonly used electron-microscopy methods. X-rays have a higher sensitivity to lattice strains and can be used to image larger areas of the specimen. Other novel applications will include time-resolved studies of plastic deformation and fracture using topographic imaging of line defects. Using high-brilliance sources, these studies will be able to determine lattice strains with a spatial resolution of a few micrometers. Experiments can be carried out in aggressive environments, and in situ studies of corrosion and oxidation will be possible.

Studies of the dynamics of phase transitions such as precipitation, solidification, and melting will be carried out by direct imaging; the same technique will be used to study the dynamics of domains in ferromagnets and ferroelectrics. Dynamic imaging of acoustic waves and of their interaction with lattice defects will also be possible, thus allowing the study of acoustic delay lines and filters.

Area-resolved EXAFS using wavelengths near an adsorption edge to form a white-beam topograph has been demonstrated and will allow correlations of the EXAFS data obtained from small-volume samples such as precipitates and grain boundaries. With extremely high-intensity sources, all these experiments could be done with a time resolution in the millisecond to microsecond range, thus making it possible to observe dynamical changes.

EXAFS and NEXAFS -- These techniques have a wide range of possible applications to metallurgical problems. Some of the more interesting possibilities involve investigation by fluorescent x-ray-absorption spectroscopy of the structures formed by relatively dilute (0.01% to 1.0%) solutes that influence the physical properties of steel and other alloys. Experiments of this type have studied internally oxidized Fe in Cu at a level of 75 ppm and have revealed that the structure differed from that of bulk oxides. Investigations of fine carbide, nitride, and carbonitride precipitates in high-strength low-alloy (HSLA) steels containing 0.05% to 0.2% Nb, V, or Ti have been carried out, and time-resolved techniques have been used to study the precipitation of Nb carbides in a steel.

Some of the many other metallurgical problems that are amenable to investigation using EXAFS/NEXAFS techniques are:

1. Investigation of the structure and chemistry of the complex precipitates that form in industrially important alloys. These studies will include the partitioning of solutes between the solid solutions and the several types of precipitates. Examples of such important precipitation systems are the complex alloy carbonitrides in HSLA steels.
2. The formation of complex oxides in stainless steels and other corrosion-resistant alloys is poorly understood. Through the use of high-intensity sources, EXAFS techniques may be applied to these problems. These measurements will be carried out in situ during oxidation or corrosion reactions.
3. Using high-intensity synchrotron sources, studies can be undertaken of the local atomic structure and chemistry of grain boundaries enriched by segregation of such elements as Sn, Sb, As, P, and S. These measurements can then be correlated with those obtained from studies of temper embrittlement in steels, of grain-boundary embrittlement in Ni-base alloys, and of hydrogen embrittlement.

Fluorescence Analysis -- New synchrotron sources offer exciting opportunities in the use of fluorescence analysis to chemically analyze micrometer-sized areas; elemental sensitivities on the order of parts per billion would be possible for many important elements, including some of the important lighter alloying elements. Additionally, the x-ray optics developed for this technique will also allow the use of EXAFS and NEXAFS techniques on micrometer-sized regions.

Small-Angle Scattering (SAS) -- New synchrotron sources will enable significant advances in small-angle-scattering techniques. These techniques will be of great importance in studying the early stages of precipitation in many alloy systems. Particularly important applications will be made to polymer studies, and some of these have already been undertaken. Real-time acquisition of small-angle-scattering patterns at a data rate of 30 Hz has been accomplished and is being applied to the study of crazing in rubber-modified polymers and glassy polymers. Many other properties of polymeric systems, particularly their behavior under applied fields, will be better understood with the advent of these new techniques.

Phase-Transition Physics

One of the major achievements of modern condensed-matter physics is the general understanding of the phase-transition problem. In the context of this basic understanding, it is remarkable that so much remains to be discovered about the mechanisms and characteristics of various phase transitions. SR techniques have made important contributions to our understanding of these subjects, particularly in the heretofore virgin area of two-dimensional structural phase transitions. Generally, these SR studies have produced higher-quality data than have been obtained using conventional x-ray and neutron sources in studies of three-dimensional systems. The advantages here of SR are: 1) intensity levels high enough to get a reasonable scattering rate from

a single atomic layer and 2) high collimation of the beam, which permits the study of structural correlations involving lengths up to 1 μm . Some of the highlights of this research are described below.

The Absence of Long-Range Order in Two-Dimensional Crystals -- On quite general theoretical grounds, two-dimensional systems, unlike their three-dimensional counterparts, cannot develop rigorous long-range order. Although this concept has been understood theoretically for a few decades, no experimental verification of these effects was possible with conventional x-ray sources or with other probes. With the development of SR-based high-resolution scattering techniques, such studies have become possible. Detailed analysis of the diffraction line shapes obtained from freely suspended liquid-crystal bilayers and from incommensurate xenon monolayers adsorbed on graphite have documented these effects quantitatively.

Two-Dimensional Melting -- Experiments designed to follow the melting process in a two-dimensional layer, with temperature resolution of a few millikelvin, have been carried out on a number of systems, including variable-thickness liquid-crystal films and krypton and xenon monolayers (see Figure 8). Systems without a substrate and incommensurate systems show both first- and second-order melting behavior; the type of melting behavior that is shown in a particular case depends on the details of the system. A new phase in two dimensions, the so-called hexatic phase, has been seen in substrate-free systems, in multilayer systems, and in systems with an incommensurate substrate.

Commensurate/Incommensurate Transitions -- The influence of a substrate potential may lead to new phases in the phase diagram of a monolayer system. Specifically, the monolayer may be perfectly registered with the surface, or it may be incommensurate. When it is incommensurate, it may have its crystal axes either aligned or rotated with respect to the substrate axes. In cases in which the substrate is biaxial, the adsorbate system may be incommensurate in one spatial direction and commensurate in the other. All of these cases have recently been seen in various systems studied with SR, and transitions between them are under active study. One of the most unexpected discoveries in this endeavor was the observation that the commensurate/incommensurate transition proceeds through an intermediate, disordered, liquid-like phase. This phenomenon may have important consequences in the growth of ordered epitaxial structures.

Multilayer Phenomena and Wetting -- The structure of multilayer systems is as important as the structure of the surface and adsorbate layers. Important questions concern the transition from the nonwetting regime, in which only a few layers will adsorb below bulk coexistence, to the wetting regime, in which an infinite number will adsorb. Remarkable phase transitions occur in which, for example, a system consisting of one adsorbed layer and of bulk crystallites transforms to two adsorbed layers with correspondingly less bulk material. So far, this behavior has been studied for ethylene and oxygen adsorbed on graphite, and a great deal of work remains to be done in many other systems.

Biological Structure

Over the past decade, SR studies have played an ever-increasing and, in some cases, pivotal role in unraveling aspects of the molecular structure and

XENON ADSORBED
ON GRAPHITE (001) SURFACE

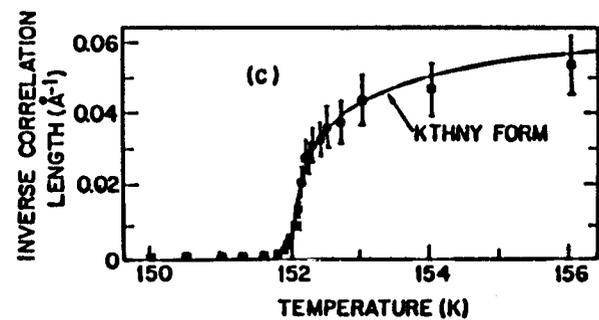
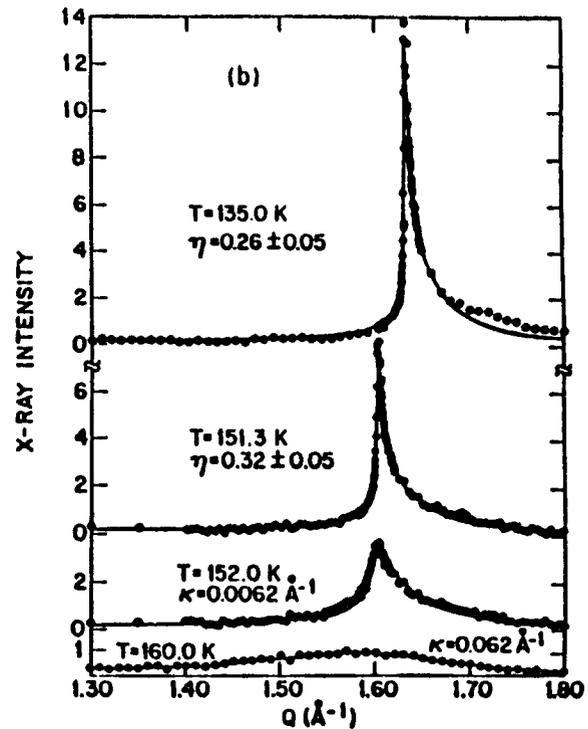
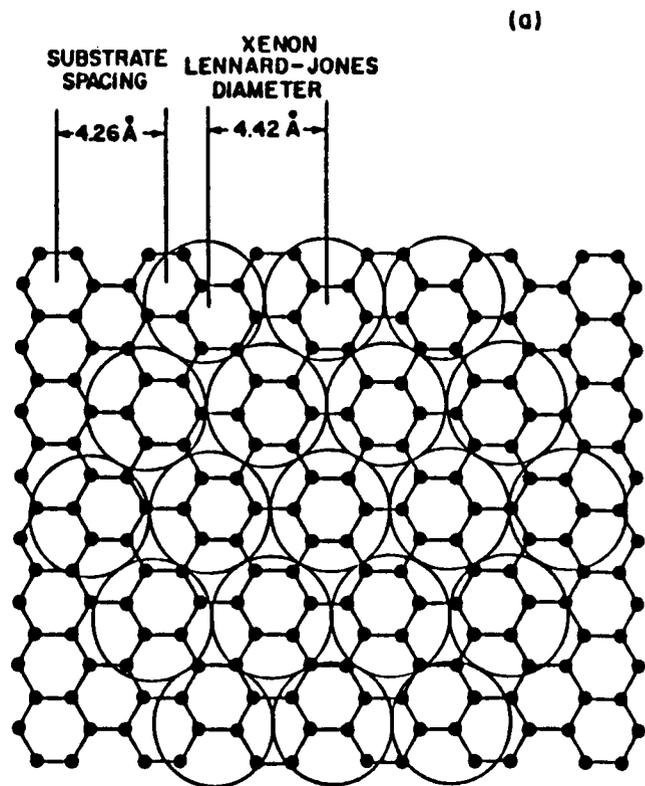


Figure 8. Melting of a Xenon Monolayer on Graphite. (a) An illustration of a monolayer of xenon adsorbed on the (001) surface of graphite. (b) Diffraction line shapes illustrating the absence of long-range order in the two-dimensional solid and demonstrating the continuous nature of the melting phase transition. (c) The measured temperature dependence of the inverse correlation length at the melting transition compared to a theoretical prediction.

function of biological systems. This has been true in studies of local structural environments of metalloproteins, using x-ray-absorption spectroscopy (NEXAFS and EXAFS); studies of macromolecular assembly and function, using small-angle x-ray scattering; and studies of three-dimensional protein structures, using crystallographic and anomalous-scattering methods.

X-ray-Absorption Spectroscopy -- The availability of SR revolutionized our ability to obtain useful information from x-ray-absorption spectra. EXAFS has proven its capability for determining the atomic arrangement around a specific atom in materials under physiological conditions. Distances can be determined to accuracies of within a few hundredths of an angstrom and coordination numbers and types can also be determined. Information about site symmetry and oxidation state is provided by edge analysis.

EXAFS and edge spectroscopy have demonstrated particular applicability to biological systems in which a metal ion is the site of catalytic action that results in the binding of a biologically active small molecule (such as dioxygen). For example, the enzyme nitrogenase is responsible for the conversion of atmospheric dinitrogen into ammonia, which can be assimilated by growing plants. Structural aspects of the molybdenum site in nitrogenase were elucidated for the first time by EXAFS (see Figure 3), thus stimulating activity toward synthesis of inorganic analogues. In chloroplasts, EXAFS has been used to help define the role of manganese in photosynthesis. Cytochrome oxidase is the terminal electron acceptor in the mammalian respiratory chain. Crucial questions about the nature of the iron and copper atoms in the enzyme have been resolved by EXAFS.

X-ray Crystallography -- X-ray-crystallographic studies provide virtually all of the information that we have about the three-dimensional structure of proteins and about how enzymes function on a molecular level. One of the most common problems in protein crystallography is obtaining crystals of sufficient size and stability to allow collection of three-dimensional diffraction data. SR studies in the USA and in Europe have shown significant enhancement in achievable resolution and significant reduction in the time required for such studies. It has also been found that some protein crystals undergo less radiation damage for a given dose if it is applied over a short time.

Recent developments in the ability to crystallize membrane proteins, using special detergents, enable the use of protein crystallography for the determination of the atomic structure of these proteins. However, a major difficulty is the production of sufficiently large crystals to obtain diffraction to a reasonable resolution. Use of high-brightness sources would allow measurements on crystals whose volume is on the order of 10^3 times smaller than the volume needed at the present time. A measurement technique capable of such resolution would find a very wide range of applications because many proteins can only be crystallized in very small sizes.

Another important technique involving the preparation of two-dimensional protein single crystals by adsorption to a lipid monolayer is opening up a new field of structure determination for biological molecules. Preliminary work has shown that it is possible to obtain well-defined diffraction peaks from adsorbed lipid monolayers on a crystalline substrate. The extension to crystals of macromolecules, such as proteins, has not yet begun. In the near future, it should be possible to repeatedly prepare $10 \times 10 \mu\text{m}$ monolayers of

immunoglobulin crystals. The use of x-ray diffraction from such samples could allow the determination of structure at high resolution, for molecules that will not crystallize as three-dimensional structures.

Anomalous X-ray Diffraction Studies -- The use of anomalous scattering is gaining importance for biological-structure studies. Normally, the classical phase problem is solved in protein crystallography by means of multiple isomorphous replacement through soaking the crystals in solutions containing heavy-metal ions. By using multiple data sets, one from each heavy-atom derivative, the structure of the protein crystal can be determined.

The same information can be obtained by changing the wavelength of the x-rays around the absorption edge of an element already present in the sample. This technique is currently proving to be very useful in obtaining direct-phase information and thereby a solution of the crystal structure. The experiments are difficult owing to the small change in total effective electron density as the x-rays are tuned through an absorption edge: for lanthanide ions these changes, some of the largest known in any element, are in the range of about 20 electrons. The resulting change in diffraction intensity in a large molecule that may contain many thousands or tens of thousands of electrons is on the 0.1% to 1% level. In order to obtain a measure of such small changes with a sufficiently good signal-to-noise ratio, a very large number of counts needs to be taken.

A very high data rate is important because radiation damage is likely caused by migration of free radicals. Thus, it is advantageous to use a very-high-brightness source in addition to taking other precautions (such as rapid cycling of the sample through the beam) to minimize the effects of radiation damage. As the sensitivity of the technique is improved, new ways of labeling specific regions of molecules of interest may be developed, for instance by means of special lanthanide chelating agents that would bind in a controlled way to specific sites in a macromolecule. Anomalous diffraction could then be used to locate the marker group within the overall molecular structure.

Small-Angle Scattering -- Small-angle scattering is useful for studying the structure of biological molecules at intermediate resolution and for following changes in the structure as a function of time. One of the earliest uses of SR was to record time-dependent diffraction from a contracting muscle. The studies yielded information about the nature of cross-bridge action in the contractile process. Studies of scattering from solution have helped define the way in which microtubules are assembled from subunits and the assembly of viral proteins into a capsid. The conformation of macromolecules in solution can also be studied as a function of biological effector.

Summary -- In summary, the availability of sources of increased brightness will open up new possibilities in the use of x-rays for biological-structure determination. The availability of an intense, highly collimated x-ray beam can be exploited in a number of ways. These all depend on selective use of the very high fluxes that can be made incident on a biological sample either in time, to give time-resolved diffraction information; in energy, to give increased ultrahigh resolution that can be used for inelastic studies; or in real space, to make it possible to get useful diffraction information from ultrasmall samples. The combination of high brightness and tunability available in an SR x-ray source will also make possible the use of anomalous x-ray diffraction on samples involving high dilution of an anomalous scatterer.

Medical Applications of SR

In the U.S. there are about 3-1/2-million people who suffer from symptomatic coronary-artery disease and about 1-1/3-million new heart attacks per year, half of which are fatal. Screening high-risk subsets of the population is currently ineffective because the tests are too insensitive, too risky, and too costly. The present reference standard for assessing the extent and the severity of coronary disease is the invasive coronary arteriogram, in which a catheter is inserted through an incision and an iodine-containing contrast agent is injected into the artery; radiographs, including cine images, are then recorded.

The properties of SR make it highly suitable as an x-ray source for use in a relatively safe and inexpensive approach based on iodine K-edge dichromography. A rapid scanning procedure is performed in which pairs of line images are recorded with monochromatic radiation above and below the K-edge of iodine (33.16 keV). The logarithmic subtraction of the two recordings results in an image whose sensitivity to iodine is about 39,000 times greater than it is to bone and about 170,000 times greater than it is to soft tissue. Preliminary recordings of the central circulation in anesthetized dogs provide good images of the major vascular structures and have demonstrated one of the coronary arteries, the left anterior descending artery, whose diameter in a dog is typically about 1 to 2 mm.

What will happen if future experiments on humans are successful? There is a high probability that there will be the need to develop compact, inexpensive, and widely available SR sources. These can also be used for other medical purposes. For instance, barium K-edge (37.44 keV) dichromography could result in a reduction in x-ray dose and in an increased information yield in studies of the gastrointestinal tract. A similar approach can be used for nonangiographic iodine-based procedures such as myelography, cholecystography, and urography. The extreme sensitivity of the K-edge dichromographic technique to iodine will allow a major reduction in contrast-agent dose in those patients who cannot tolerate conventional doses. Such patients include the elderly and patients with severe hypertension, poorly controlled diabetes, renal failure, and other disorders. Finally, tunable monochromatic imaging could increase contrast in any form of radiography, thus improving the information yield for a given radiation dose.

Catalysis

Heterogeneous catalysts represent one of the most complex class of materials that have been studied with x-ray-absorption spectroscopy. These materials can be classified broadly as either metallic or nonmetallic catalysts, and in both cases the catalytic components are generally distributed on high-surface-area insulating supports. Supported metallic heterogeneous catalysts have been more widely studied with x-ray-absorption spectroscopy, but nonmetallic systems (mostly oxides and sulfides) have received some attention. Both types of catalysts are important technological materials, and numerous industrial processes in the petroleum and chemical industries are dependent on them.

Supported Metal Catalysts -- The early EXAFS studies of supported metal catalysts were initiated in the period (mid 70s) when EXAFS was in its infancy.



Figure 9. An Example of K-edge Dichromatography of the Arterial Structure of a Pig's Heart. Logarithmic subtraction of line images taken above and below the iodine K-edge yields greatly enhanced sensitivity to the arterial structure and discriminates against bone and soft tissue. Successful experiments have been carried out on anesthetized dogs.

The early work focused primarily on the structure of supported monometallic catalysts and for the first time provided catalytic chemists with detailed structural information on the small metal clusters that comprise these catalysts. Studies of the more complex supported bimetallic catalysts were undertaken following the early work on monometallic systems. Techniques were developed for analyzing these systems, and there is now a growing body of literature concerning the structure of these mixed-metal clusters. This work also contributed to the general development of EXAFS as an analytical technique by providing a body of structural information that could be assessed and compared to information from established catalytic-characterization techniques such as chemisorption, probe reactions, and electron microscopy.

Studies Under Reaction Conditions -- The use of SR for x-ray-absorption-spectroscopy studies of catalyst systems while reactions are actually occurring is an exciting development. The feasibility of such studies has already been demonstrated, and the resultant measurements will undoubtedly receive increased emphasis in the future. The possibility of relating the activity of a catalyst to structural and electronic properties of the catalytic system under reaction conditions is now at hand, and one can anticipate that such research will lead to a greater depth of understanding of catalytic phenomena.

With further experience in the use of SR in the study of catalysts and catalytic phenomena, one can anticipate that the volume of research will increase markedly. Although studies to date have been concerned primarily with basic-research programs on catalysts, an increased awareness of SR as a valuable tool in process- and catalyst-development programs in industry can be anticipated.

Zeolite Catalysts -- The activity and selectivity of zeolite catalytic materials are largely governed by their framework structures. Detailed structural information is then the key to understanding the properties of zeolitic materials. Unfortunately, most zeolites cannot be made in crystal sizes sufficiently large for conventional single-crystal x-ray structure analysis. Quantitative structural information is then only accessible through the use of powder-diffraction data. The averaging of the three-dimensional information limits the precision with which the structure can be defined.

High-brightness sources present the opportunity of accessing single-crystal diffraction data from very small particles--Micro-crystal Diffraction. In the first measurements obtained with this technique, data were taken from two cancrinite crystals with volumes of 13,000 μm^3 and 800 μm^3 respectively. These data demonstrate the feasibility of the technique and indicate that complete diffraction-data sets from micrometer-sized crystals should be routinely accessible. Owing to the severe limitations inherent in the use of powder data for structure solution, the application of synchrotron x-radiation in Micro-crystal Diffraction is expected to provide novel structural information on many catalytic materials, notably zeolites.

Earth Sciences

The application of SR to problems in the earth sciences is just beginning. It is clear that the many new studies that are possible with SR but not possible with conventional laboratory photon sources will have both substantial impact

in the earth sciences and important technological applications. Although the growth of this synchrotron effort has been severely limited by a lack of available beam time, a number of investigations have highlighted the areas in which exciting results can be obtained. The major applications to date mainly involve x-ray-absorption and -scattering studies.

Structure and Composition of Silicate Glasses -- The major purposes of this effort are to derive interatomic distances, coordination numbers, and concentrations for various elements in amorphous silicates. This work will improve understanding of structure/composition-dependent melt properties such as viscous flow, cation diffusion, and the solubility mechanism of volatiles (H_2O , CO_2) in silicate melts. Future work in this area will involve study of trace levels (<0.1%) of rare-earth, lanthanide, and actinide elements in silicate glasses and crystalline model compounds. In terms of geological importance, these studies have bearing on magma transport, eruptive mechanisms, crystal-melt element partitioning, element segregation in magma chambers, and melt growth of crystals. For certain glass compositions, these studies will also have bearing on nuclear-waste disposal.

Aqueous-Metal EXAFS -- This work has focused on the structure of metal complexes in concentrated aqueous solutions and on how this structure varies as a function of pH and ionic strength. Systems studied to date include electrolyte solutions involving Cr, Fe, Ni, Cu, and Zn cations and Cl and Br anions. Fluorescence EXAFS studies of ZnCl solutions at concentrations as low as 0.0001 M have been carried out. These concentrations approach those in natural hydrothermal solutions and in sea water, thus making it feasible to carry out speciation studies on the types of complexes that transport metal ions such as Fe, Ni, Cu, Ag, Au, and U in hydrothermal fluids emanating from cooling magma bodies and from midocean-ridge hydrothermal systems. These types of hydrothermal solutions are thought to be responsible for the transport and deposition of metalliferous ores that are so critical to our economy. Future work on geochemically important solutions should involve EXAFS studies at temperatures in the hydrothermal range (100° to 350°C). Our knowledge of the types of complexes present in heated solutions is currently limited to indirect information derived in part from solubility measurements. An important application of high-temperature (<100°C) EXAFS studies of aqueous complexes will be the study of radionuclide complexes such as those that could escape into heated groundwaters surrounding geologic waste-disposal sites.

High-Pressure/High-Temperature Phase Transitions and Equations of State

-- One of the earliest applications of synchrotron x-ray work to geologic materials involved crystallographic studies of phases held at high pressure in diamond-anvil devices. With current technology, pressures as high as 1.7 Mb can be generated and held by such devices, permitting geochemists to model phases that might occur in the earth's lower mantle and outer core. Recently, simultaneous heating of pressurized samples has been accomplished to determine the equations of state of mantle materials. Because of the thickness of the diamond windows necessary for such experiments and because of the need for rapid measurements, these experiments are best done using synchrotron sources. Future work will involve scattering studies of oxides and silicates at pressure, in order to determine elastic constants. An exciting evolution of the current high-pressure/high-temperature phase-transition work involves time-dependent studies of the kinetics of phase transitions. One of the key theories developed recently for deep-focus earthquakes near plate boundaries involves mantle

phase transitions. However, questions concerning the kinetics of such transitions must be answered before these theories can be fully evaluated.

Powder-Diffraction Studies — Many geological materials occur in such small particle size that conventional structural characterization involving single-crystal techniques is not possible. Similar difficulty is faced with many synthetic materials, particularly those quenched from high pressures, that are used to model chemically more complex natural analogues or phases that may occur deep in the earth's interior but that are not naturally present in crustal rocks. Profile fitting of high-quality powder-diffraction data of such phases is essential for their structural characterization. Preliminary synchrotron studies have shown significant gains in resolution relative to the resolution obtainable using conventional sources; these gains will permit considerably more complicated structures to be studied. Future applications of powder-diffraction studies include phase-transition studies and the study of order/disorder relationships in minerals.

X-ray-Microprobe Analysis — There is a critical need to improve the detection limits for trace elements in geologic samples, while maintaining high spatial resolution for in situ analyses. The electron microprobe has revolutionized the study of materials, including those that occur naturally, and is capable of detecting elements with Z greater than 5 in amounts as low as 0.05 weight percent, with a spatial resolution of several square micrometers. Plans are underway to construct an x-ray analogue of the electron microprobe. Preliminary work has already shown that current technology is capable of producing a microprobe with minimum-detection levels of 1 to 10 ppm/s/m and a bulk-analysis system with a sensitivity of 30 to 100 ppb in a 1-minute irradiation. In situ measurement of trace elements will permit the study of trace-element partitioning among phases. Such data are essential for unraveling the origin of magmas and for studying their crystallization histories.

Structural Characterization of Metamict (Radiation Damage) Materials -- A number of important geologic phases commonly occur in the metamict state due to the structural damage caused by the decay of radionuclides present in small amounts. An important example is the abundant mineral zircon, $ZrSiO_4$. These heretofore poorly characterized phases to some of the crystalline and amorphous materials proposed as hosts for waste radio-nuclides. The benefit of studying naturally metamict materials derives from the fact that the metamictization process in these materials has proceeded at natural rates, which are much slower than those realizable in the laboratory but which are similar to those that would occur in nuclear-waste repositories. Anomalous-scattering radial-distribution function (RDF) studies of these materials will also yield structural data that are complementary to those obtained using EXAFS.

Other Applications — Many other applications of SR to earth-science problems are possible within the next few years. Some important examples of such applications are: (1) x-ray-adsorption studies of melts, (2) characterization of mineral surfaces, including adsorption and desorption properties, using the surface techniques made possible by synchrotron sources, (3) the study of melting phenomena involving minerals, (4) the application of anomalous-scattering methods in the study of amorphous and metamict silicates, (5) the study of phase separation in geologic systems, using small-angle x-ray scattering, (6) single-crystal diffraction studies with superior signal-to-noise ratios and involving very small crystals, and (7) time resolution of transient effects such as those occurring during melting and during reactions of mineral surfaces with water and gases.

Plasma Physics

Plasma physics is an area with important defense, energy, and materials-technology implications. Studies of the optical properties of dense, hot (10^6 to 10^7 K) plasmas in the soft x-ray region have been very limited due to the high intrinsic brightness of the plasma. The ability to study hot and warm atoms and ions in both equilibrium and nonequilibrium conditions is crucial in the design of devices based on plasma interactions. Such devices are used in energy research, in the development of inertial- and magnetic-confinement fusion; in defense technology; in the study of such problems as arc formation in electrical switches and in flashover phenomena; and in the development of various plasma surface-processing techniques.

Undulators on a machine such as the Advanced Light Source (ALS) would produce x-rays that are unusually brilliant in the prime area of interest (100 to 1000 eV). In this energy range, the peak brilliance of the radiation from such an undulator would be greater than that of the radiation from a 1-keV Planckian, and this brilliance would make it possible to conduct studies on warm and hot atoms that heretofore could not even be contemplated. Above 10 keV even the radiation from wigglers on such a machine would be more brilliant than most laboratory-produced plasmas, and the radiation from undulators on a 6-GeV machine would far exceed the plasma in brilliance.

The new generation of SR sources would be very useful in the detailed study of dense plasmas. Diagnostics to measure Doppler broadening and even classical plasma interferometry would be possible, and measurements could be made at much higher frequencies than is currently possible. Plasmas with electron densities in the 10^{25} to 10^{27} e/cm³ range would be transparent to x-rays at these frequencies (100 to 1000 eV), and thus undulator beams could be used as back-lighting sources. The beams could also be used to study bound/bound and bound/free absorption by highly ionized atomic species. Details of ionic populations could be measured, and x-ray-absorption coefficients of "warm" or "hot" atoms could be studied in detail.

Owing to the short pulse length and the high degree of linear polarization of these beams, the signal-to-background ratio could be substantially improved from the ratio attainable with conventional methods, which employ laser-produced plasmas to emit copious amounts of line radiation at restricted energies. Finally, the high brilliance of the new sources makes it possible to obtain the high spatial resolution required to perform such measurements as those described above.

Actinide Chemistry

The actinide or transuranium elements from Th to Lr constitute the least-understood chemical series due to their variety and high radioactivity. They are also, of course, of central importance in nuclear-energy development, nuclear-waste disposal, and nuclear-weapons technology. However, especially for the heavier elements of this series up to Es, the quantities available for study may be only in the milligram to microgram range. Effective source sizes are thus only 0.2 to 0.5 mm in diameter, with samples often being prepared in small capillaries. The extreme radioactivity of these materials also dictates that the sample be placed at least 1 meter from an external radiation source so that adequate safety shielding can be present.

Thus, although it is clearly of high interest to better study these elements and their compounds--for example, by photoelectron spectroscopy and other related techniques--achieving adequate intensities will require a special radiation source, particularly one with high brilliance in the VUV/XUV range. A source of sufficiently high brilliance could yield a beam of the requisite 0.2 to 0.5-mm diameter even at distances greater than or equal to 1 meter from the monochromator and could thus illuminate the specimen with full efficiency. It is estimated that such brilliances would have to be higher by a factor of from 10^2 to 10^4 than those of presently available SR sources, so that a highly optimized undulator-based source is suggested, such as those planned for the ALS. The optimum range of photon energy would be 20 to 600 eV so as to permit studying both valence (5f, 6d, 7s) and core (4f, 6p) levels.

Such a source would permit studying the gas-phase elements, the solid elements, and their compounds. Gas-phase atomic studies would provide an important reference point in determining the detailed electronic structure and in assessing the very strong relativistic effects involved. The rich multiplet structure expected in valence- or core-photoelectron emission from these elements would also require resolutions less than or equal to 0.1 to 0.5 eV to adequately resolve the features expected.

The types of measurements feasible would then include UV and soft x-ray photoemission, possibly in an angle-resolved mode. Two closely related photoemission measurements that could be performed are CFS and CIS spectroscopy. In the first of these techniques, a constant final state photoelectron energy is used with swept photon energy to map out initial-state density; in the second technique, a constant initial state energy is used with swept photon energy to map out final-state density. These materials would also be expected to exhibit "resonant photoemission," in which the photoelectron intensity from a given level exhibits abrupt changes as photon energy is swept through the binding energy of a lower-lying level; such measurements would provide very subtle information on the valence-state configuration and the valence/core interactions in those materials.

In compounds, it also would be of interest to do core-level EXAFS in order to determine bond distances. Particular features of the actinides that would be of interest include the atomic number at which the relatively weakly bound valence 5f electrons change so as to exhibit the behavior of the more strongly bound valence 4f electrons in the rare earths. Density-of-states measurements in solids, by means of photoemission, also would be of interest in locating the 5f levels, which lie very near the Fermi level. Finally, these materials might be expected to exhibit a different divalent state near their surfaces; this possibility could also be studied with these SR techniques.

In conclusion, studies of this very important and very poorly understood series of elements would be significantly enhanced by the availability of a next-generation VUV/XUV undulator source with high brilliance.

FACILITIES (USA)

Introduction

This section is divided into five major parts dealing with existing facilities, future facilities, cost projections for the development of future facilities, users, and important research and development (R&D) efforts that relate to synchrotron radiation (SR) facilities. The status of foreign SR facilities is described in Appendix B.

Existing Facilities

SR facilities in the USA that are in operation or are being commissioned are listed in Table 3 below.

Table 3

Existing SR Facilities in the USA

<u>Institution</u>	<u>Name of Machine</u>	<u>Operating Energy</u>
National Bureau of Standards	SURF II	0.28 GeV
University of Wisconsin, SRC	TANTALUS	0.25 GeV
University of Wisconsin, SRC	ALADDIN	0.75 to 1 GeV
Stanford University, SSRL	SPEAR	3 to 3.5 GeV
Cornell University, CHESS	CESR	5 to 5.5 GeV
Brookhaven National Laboratory, NSLS	VUV	0.75 GeV
Brookhaven National Laboratory, NSLS	XRAY	2 to 3 GeV

The following is a brief description of each of these facilities, giving the status of each as of the fall of 1983 and the individual plans for further development.

National Bureau of Standards--SURF II

SURF II is the USA's longest-operating synchrotron light facility, and it has some unique features. Unlike the other rings in the country, the electron orbit in SURF II is circular because it is contained between the poles of a single magnet. This circular electron orbit gives SURF II the capability of operating as an absolute-standard light source with which, given knowledge of the beam energy and position distribution in the orbits, the absolute intensity of the SR as a function of wavelength can more easily be calculated. The SURF II staff estimates that this calculation can now be done to an accuracy of 2% at a wavelength of 200 nm and to an accuracy of 3% at 4 nm. This accuracy is

FACILITIES (USA)

better than that required for the calibration of, for example, spectrographs used in astronomical research.

SURF II operates at 0.28 GeV with an initial current of 30 to 60 mA. Machine improvements over the last year in the rf, in the power-supply regulation, and in the vacuum are responsible for an increase to the present current level and an increase in beam lifetime. New monochromators emphasizing resolution and throughput are coming on line, as is a new high-resolution, angle-resolved electron spectrometer that is designed for use in gas-phase spectroscopy. This spectrometer involves a twice-standard-size spherical analyzer with improved throughput at high resolution, and it employs three layers of magnetic shielding. There are currently eight experimental stations, with three more due on line next year.

University of Wisconsin--SRC (Synchrotron Radiation Center)

This laboratory has the 0.25-GeV ring TANTALUS, which has been in operation for some time, and ALADDIN, a 0.75 to 1-GeV ring that is now being commissioned.

In recent years TANTALUS has operated at a level of 95% of its scheduled time, which represents extreme machine reliability. The facility has been remarkably "user friendly" and serves as a model for other user facilities. Some of this success may be a matter of scale and thus may be difficult to maintain at the larger facilities characteristic of the future.

Like the vacuum ultraviolet (VUV) ring at the National Synchrotron Light Source (NSLS), the ALADDIN ring is designed as a second-generation SR source for research in the VUV and soft x-ray regions. It is designed with a low-emittance lattice that will give enhanced brightness to the bending-magnet source points, and it has four long straight sections (4 meters in length), of which at least two will be available for future insertion devices such as wigglers and undulators. This ring is now being commissioned, and many subsystems are being completed or developed. The 100-MeV Microtron injector is operating, and low-current beams have been injected into the storage ring and accelerated to 0.75 GeV. There are potentially 35 ports that can be developed from bending-magnet source points, and approximately 23 beamlines are now being developed.

Most of the eight monochromators now operating on TANTALUS will be shifted over to ALADDIN as part of the 23 devices that will be available in its early stages of operation. About half the monochromators belong to participating research teams (PRTs), and the other half are built and operated by the facility. A number of the new ALADDIN monochromators will operate in the difficult photon regime of several hundred to several thousand electron volts.

Stanford University--SSRL (Stanford Synchrotron Radiation Laboratory)

This is the largest of the presently operating U.S. synchrotron light facilities, and until the advent of CHESS, it was the sole source of harder x-rays. The SPEAR storage ring was built as an electron-positron colliding-beam machine for high-energy-physics research, and it continues to operate in this mode 50% of its operating time. (SPEAR currently operates a total of eight months out of the year.) When SPEAR is dedicated to high-energy-physics research, SSRL operates on a parasitic basis, and the beam energy ranges from

1.5 to 2.5 GeV, with beam currents of 5 to 25 mA. The remaining time the ring is operated in a dedicated mode for SSRL at beam energies of 3 to 3.5 GeV and with a typical current of 100 mA and a beam lifetime of between 10 and 20 hours.

SPEAR has many 2-meter-long straight sections that were originally used for beam-diagnostic and control equipment. Over the past several years, a program of modifications to the storage ring has made many of these straight sections available for insertion devices, and SSRL has pioneered the use of wigglers and undulators in such locations. There are now two 8-pole, 18-kG wigglers, a 60-pole variable-gap undulator, and a 54-pole variable-gap wiggler. The last two devices were constructed in collaboration with Lawrence Berkeley Laboratory (LBL).

Cornell University--CHESS

This facility operates parasitically on the high-energy electron-positron storage ring CESR, which typically runs at beam energy of 5 to 5.5 GeV. CHESS is the source of the hardest radiation available in the United States. There are six experimental stations, each accepting 14 mrad of light, on three beamlines. Until recently, typical currents were 15 to 20 mA, but recent modifications allow multibunch operation, and 75 mA in three bunches 870 ns apart is now anticipated. The bunches are very short (130 ps), and much of the research at Cornell has made use of this time structure in time-dependent studies.

A six-pole, 18-kG wiggler station is currently being implemented at CHESS. On it will be a carousel monochromator spanning 4 to 60 keV and a line for Bragg-Laue crystallography. In addition, there will be a large four-axis Huber instrument for accurate structure-factor measurements and for the electron-density mapping of crystals. Hard radiation will be employed for these studies so as to reduce the importance of extinction corrections.

Brookhaven National Laboratory--NSLS

The NSLS at Brookhaven National Laboratory is the first dedicated SR source in the U.S. with storage rings individually optimized for high brightness in the x-ray and ultraviolet (UV) regions. It is a national user facility, with user groups organized principally into PRTs; these PRTs have committed substantial resources and personnel to the construction and operation of beamlines on which they will utilize up to 75% of the operating time. (The remaining time is available to general users.) Representation in these PRTs includes 28 groups representing universities, industrial laboratories, and government laboratories.

The NSLS Phase I was a four-year construction project that began October 1, 1977. Groundbreaking occurred in September, 1978, and startup of the VUV ring took place late in 1981. Research at the VUV ring was underway by mid-1982. The XRAY storage ring is now in the commissioning stage and is expected to provide photons to users within the next few months.

The VUV storage ring is a four-superperiod machine of 51-meter circumference. Its principal design parameters are an energy of 700 MeV and a

circulating beam current of 1 A. It now operates at 750 MeV and has achieved a peak beam-current value of 300 mA and a source-brightness value of approximately 4×10^{13} photons/s \cdot mm² \cdot 0.1% bandwidth. Each superperiod or ring quadrant consists of a 90-degree bend section with optical characteristics that are favorable for achieving minimum beam-emittance values and that permit greater freedom for installing undulators or wigglers in the straight sections without adversely affecting the storage-ring beam parameters.

The four connecting long straight sections (each 3.2 meters in length) are used as follows: One is used for beam injection, one is used for an rf station, and two are used for insertion devices. One of these last two sections is now used for a 38-pole permanent-magnet undulator, which has been installed and operated and which is now being instrumented for usage in the 100 to 1000-Å range. It provides for a potential brightness increase, compared with a VUV bending-magnet arc source, of approximately a factor of 100.

The photon beams are transported from each VUV-ring bending magnet, with a radiation fan of 75 to 90 mrad. The fluence is approximately 10^{14} photons/s \cdot mrad \cdot 1% ($\delta\lambda/\lambda$) at the critical wavelength of about 25 Å (750 MeV). Under design conditions, the maximum source brightness at approximately 1-keV photon energy is 3×10^{14} photons/s \cdot mm² \cdot 1% ($\delta\lambda/\lambda$) for the VUV-ring-arc source. There are presently 13 ports being used or developed, and they split into two or three beamlines. By the end of 1983, there should be 18 beamlines in use or being commissioned, with 6 more under construction.

The thresholds for the various modes of instability for the NSLS rings have been calculated, and corrections have been designed. The dominant instability mode now encountered in the VUV ring is the longitudinal coupled-bunch instability mode, caused by the beam in conjunction with the rf-cavity parasitic-mode impedances. Therefore, a one-or-three-bunch mode of VUV-ring operation has been established, which, for one-bunch operation, results in a (present) maximum current of 300 mA but also in greatly improved beam stability and source brightness. Future improvements in the source emittances should result from a resurvey and realignment of storage-ring magnets during the next long shutdown, and the overall current values should improve after a tune-splitting cavity is installed this winter.

The XRAY ring, which is 170 meters in circumference, is similar in optical design to the VUV ring. However, it is comprised of eight achromatic bend sections, thereby providing a greater number of straight sections for insertion devices. The operating energy will be 2.5 to 3.0 GeV, and studies are in progress regarding the use of a new booster synchrotron to raise the injection energy to the operating energy. The XRAY ring has already operated at up to 2 GeV in beam energy with modest beam lifetime and beam current. A commissioning program is in progress to enhance the beam intensity and to align the external photon lines with the photon fans emerging from the XRAY ring. Seventeen front ends are operational, and 25 "hutches" are assembled and are being outfitted with experimental equipment.

The maximum radiation fan in an x-ray port is 50 mrad, which is typically subdivided into two or three beam lines. The maximum integrated photon flux for the XRAY-ring design parameters of 2.5 GeV and 0.5 A is 3×10^{15} photons/s \cdot 1% ($\delta\lambda/\lambda$) \cdot 0.5A at the critical wavelength, for an arc source, of 2.5 angstroms. A superconducting wiggler at 50 kG would extend the spectrum into the hard x-ray

region with a flux (at a photon energy of 100 keV) of 10^{14} photons/s \cdot mrad \cdot 1% ($\delta\lambda/\lambda$) at 500 mA.

General Summary

There continues to be rapid growth in the number of facilities coming on line for research in both the VUV and x-ray regimes. Although the needs of the community are for more sources at all energies, there will be larger increases in the number of beamlines for VUV and soft x-ray research.

The new facilities, including insertion devices on existing machines, will make available much brighter sources than those of the past. This progress, combined with the technological development of beamline design and instrumentation, is opening up new fields of research and enhancing the capability for research in the many areas of science that presently use SR.

Some of these facilities are taking longer to become operational than the SR community had expected. The problems have not involved technical considerations but rather a lack of resources, both manpower and money. Although the rings being built are physically smaller than those built for high-energy physics, they are equally complex and technologically challenging. To build and commission them on an expeditious schedule requires not only adequate funding but also a larger well-managed team of accelerator physicists and engineers than has been available on some recent projects.

Future Facilities

The following table lists the new U.S. SR facilities that are being constructed, have been proposed, or are being designed or considered.

Table 4

Future SR Facilities in the USA

Funded and under construction

Brookhaven National Laboratory Stanford University Stanford University, SSRL	NSLS Phase II 1-GeV FEL storage ring SSRL Enhanced Photon Flux Facility (SEPPF)
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Active Proposals

Lawrence Berkeley Laboratory	1.3-GeV Advanced Light Source (ALS)
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Under Design or Consideration

Brookhaven National Laboratory Stanford University, SSRL Cornell University, CHESS	NSLS Phase III 6-GeV Facility 6-GeV-Ring Facility High-Energy Ring
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These projects are described briefly in the following, in the order in which they appear in the table.

Brookhaven National Laboratory--NSLS Phase II

The NSLS Phase II Construction Project is made up of two basic components: 1) beamline construction, involving the development and installation of at least six additional beamlines and associated insertions; and 2) conventional construction, involving expansion of the existing NSLS building. Briefly, the objectives of the project are to:

- design and build six state-of-the-art beamlines with emphasis on wiggler and undulator insertions
- provide laboratory and experimental support areas to accommodate up to 80 beamlines
- provide integrated work and office space for 128 NSLS personnel.

Proposed Insertion Devices and Experimental Beamlines -- Six beamlines and three insertions* will be designed and built as part of the Phase II Construction project (Table 5). The locations of these beamlines and insertions on the XRAY and VUV storage rings are noted in the table. The first three beamlines in the table were proposed to the scientific community as pertinent to the community's current needs and have been endorsed by the Users' Executive Committee. The NSLS Department Chairman has approved them for early construction. The remaining three beamlines will be reviewed by user groups and then approved for construction by the NSLS Department Chairman no later than July 1984.

Table 5

Experimental Beamlines and Insertions,
NSLS Phase II Construction Project

<u>Beamline</u>	<u>Insertion Device</u>
Superconducting wiggler	Superconducting wiggler
High-Q-resolution x-ray	Hybrid wiggler
X-ray microscopy and holography	Soft x-ray undulator
Infrared	None
TOK soft x-ray	Multipole wiggler
High-Energy-Resolution inelastic x-ray scattering	Hybrid wiggler

Stanford University--1-GeV FEL Storage Ring

This 1-GeV storage ring has been designed specifically for the study of free-electron lasers (FELs) and is not primarily planned to be used as an SR source. However, the present design includes locations for up to four insertion devices, and SR research in the soft x-ray region and basic accelerator-physics research are planned as secondary uses.

Stanford University, SSRL--SSRL Enhanced-Photon Flux Facility (SEPPF)

In addition to a plan to increase the number of beamlines from both bending magnets and insertion devices over the next several years, there are several other improvement programs underway as part of SEPPF. They include: (1) machine lattice modifications that could reduce the dedicated-mode beam emittance by a factor of three, thereby increasing the brightness from all sources; (2) changes in the beam-control systems, to improve the stability and control of the electron orbits; (3) construction of a new alternate injector using only a small

*The superconducting wiggler has already been constructed. The transverse optical klystron (TOK) insertion magnet will be built with non-NSLS funds.

fraction of the Stanford Linear Accelerator Center (SLAC) linear accelerator. This new injector will allow the running of SPEAR in the dedicated mode during shutdowns in the SLAC high-energy-physics program, thus providing a 50% gain in running time; (4) construction of additional office space and assembly areas; and (5) the addition of an undulator to the PEP electron/positron storage ring.

The PEP storage ring is operated by SLAC for the study of elementary-particle physics. In its present configuration, it can be usefully run at an energy of from 8 GeV to 18 GeV, although the majority of the program has focused upon activities at 14 GeV. During the normal running of the machine, the electron and positron beams emit SR from within the bending magnets with photon energies in excess of 100 keV.

More important to the SR community, however, is the fact that there are six 4-meter-long "symmetry straight" sections, many of which can accommodate wiggler or undulator magnets. In fact, three of the straight sections have 2-meter wiggler magnets already installed for the purpose of increasing the machine luminosity at low machine energies. The plan is to install in the first of these sections (symmetry straight #5) a 2-meter undulator in tandem with the existing wiggler magnet. Should the machine be run in a low-energy configuration, the diffuse wiggler radiation will be superimposed, to some extent, upon the undulator radiation, but this should create no unwanted background.

The design parameters were chosen to produce 12-keV radiation at the nominal PEP operating energy, 14 GeV, but the undulator will also produce extraordinary brightnesses at both lower and higher machine energies, as illustrated in Table 6.

Table 6

PEP-Beam-Facility Design Parameters

Electron Energy (GeV)	Electron Current ^a (mA)	Electron Emittance ^b (m·rad) ²	Fundamental Energy (keV)	Photon Flux ^a (sec ⁻¹ · [100%BW] ⁻¹)	Spectral Brilliance ^c (sec ⁻¹ [100%BW] ⁻¹ · mm ⁻² ·mrad ⁻²)
10.0	20.0	0.273x10 ⁻⁷	6.080	2.87x10 ¹⁶	2.66x10 ¹⁸
12.0	24.0	0.567x10 ⁻⁷	8.755	3.45x10 ¹⁶	1.54x10 ¹⁸
14.0	28.0	1.050x10 ⁻⁷	11.917	4.03x10 ¹⁶	1.09x10 ¹⁸
16.0	32.0	1.791x10 ⁻⁷	15.565	4.60x10 ¹⁶	0.65x10 ¹⁸
18.0	36.0	2.869x10 ⁻⁷	19.699	5.17x10 ¹⁶	0.46x10 ¹⁸

^aFor dedicated operation, increase by a factor of 3.3
^bFor dedicated operation, increase by a factor of 9
^cFor dedicated operation, increase by a factor of 3.3 x 9 = 30

The first component of the beamline is the undulator, whose specifications are given in Table 7. Its design will be the hybrid samarium, cobalt, and steel design originally developed by Halbach. The vacuum chamber will be of the fixed-gap design, with an interior aperture of 36 mm and an overall thickness of 45 mm. The undulator will have a variable gap ranging from a minimum of 45 mm to a maximum of 100 mm.

Table 7

Specifications for the PEP-Beam-Facility Undulator

Magnet gap	45 mm minimum (variable)
Electron aperture	36 mm (fixed)
Magnet period	72.58 mm
Peak magnet field	2.239 kG (maximum)
K parameter	1.518 (maximum)
Material	SmCo, steel

The beamline will immediately be ready for high-resolution scattering and diffraction experiments. It should be noted, however, that the unique properties of the PEP-undulator radiation will make it possible to explore, as research-and-development projects, alternative configurations that will optimize the beamline for, e.g., Mossbauer diffraction and high-energy-resolution x-ray scattering.

The schedule calls for the approximately 3000-ft² building (and the interconnecting beamline tunnel) to be built during the PEP summer shutdown in 1984; the beamline components will be installed in the summer of 1985.

Lawrence Berkeley Laboratory--1.3-GeV Advanced Light Source (ALS)

The design of the ALS has been optimized to achieve two major goals: to provide intense photon beams in the energy range of from 0.1 to 5000 eV and to provide very short pulses (20-ps duration) of synchrotron light for the many experiments that are performed in this energy range and that involve timing requirements. At a reduced flux, pulses of as short as 5 ps could be available under certain operating conditions. The use of a superconducting wiggler could provide useful fluxes of photons at higher energies, e.g., 40 keV.

To meet these design goals, the electron beam has a very small design emittance ($7 \times 10^{-9} \pi \text{ m} \cdot \text{rad}$), and the ring has twelve 6-meter-long straight sections for wigglers and undulators. The low emittance, which is an order of magnitude smaller than that of existing machines, makes it possible to optimize performance from the undulators in the soft x-ray region and to minimize power loading on optical components in the beamlines.

All told, 30 or more photon beamlines (user ports) would emanate from the ALS's complement of 12 insertion devices, and a comparable number of beamlines could originate in bending magnets. According to the proposal, half of the insertion devices and beamlines would be built as part of the main construction project, with the remainder being developed by affiliates or PRTs. Table 8 summarizes the parameters of the ALS design, and Table 9 gives the project cost estimates. The insertion devices included in the project costs are listed in Table 10.

LBL has had a pioneering role in insertion-device development and has done a great deal of work in beamline design relating to the ALS and to the problems

associated with very high brilliance and high power density. The laboratory has recently formed the Berkeley Center for X-Ray Optics, where these problems, along with the development of x-ray instrumentation, will be intensively pursued. LBL has a large, highly qualified team of machine physicists, engineers, and technicians; they have had an important role in synchrotron development in this country.

Table 8

ALS Design Parameters

INJECTION	50-MeV Linac 1.3-GeV Booster
STORAGE RING	Design current (400 mA) Beam lifetime (> 8 h) Emittance (7×10^{-9} π m ² rad) Filling time (approximately 3 min) 12 (6-meter) straight sections (> 30 branch lines possible) 24 bending magnets (>30 branch lines potential)
GENERAL-USER PHOTON BEAMLINES (Construction Project)	4 undulators 2 wigglers 14 branch lines

Table 9

ALS Construction Cost Estimates^a
(In FY83 Millions of Dollars^b)

Accelerator systems		26.5
Storage ring	11.7	
Injector	7.2	
Control system	2.6	
Contingency	5.0	
Beamline systems		26.4
Insertion devices	7.2	
Photon beamlines	14.2	
Contingency	5.0	
Conventional facilities		10.4
Removals and site preparations	2.2	
Building addition	2.7	
Shielding	1.8	
Utilities	2.4	
Contingency	1.3	
TOTAL		63.3

^aIncluding project management, engineering, and design costs

^bDoes not include escalation

Table 10
Summary of Currently Planned ALS
Insertion Devices (1.3 GeV)

<u>Name</u>	<u>Insertion-Device Type</u>	<u>Peak Field (tesla)</u>	<u>Period (cm)</u>	<u>Number of Periods</u>	<u>Length (meters)</u>	<u>Energy (eV)</u>
U _A	Permanent-magnet undulator	0.39	16.7	30	5	5 to 700
U _B	Hybrid undulator	0.74	6.25	80	5	25 to 1500
U _C	Hybrid undulator	0.54	5.0	100	5	75 to 3000
U _D	Hybrid undulator	0.57	3.5	142	5	200 to 5000 (>10,000 at 1.9 GeV)
W _E	Hybrid wiggler	1.60	10.0	25	2.5	0.1 to 10,000
W _F	Superconducting wiggler	5.0	14.0	14	2	1 to 10,000 (>40,000 at 1.9 GeV)

Brookhaven National Laboratory--NSLS Phase III 6-GeV Facility

NSLS Phase III includes the construction of a 6-GeV, 5-mA booster synchrotron and a 6-GeV high-brightness "undulator/wiggler" electron storage ring. This construction program is planned in two stages. The first stage involves upgrades to the existing facilities and construction of the booster synchrotron, referred to as Booster II in the following discussion. Booster II will be used as a full-energy injector into the upgraded existing XRAY storage ring. Construction of the high-energy "undulator/wiggler" storage ring will follow as the second stage of the program.

Plans for the design, siting, and commissioning of Booster II have been made in such a manner as to make use of the existing linear-accelerator and booster as the injection system. Booster II will be located where construction and commissioning will not interfere with ongoing operations.

The existing XRAY ring was designed for a maximum energy of 2.5 GeV; however, easy upgradeability to 3 GeV was allowed for. The dominant component involved in increasing the energy to 3 GeV is the addition of rf acceleration stations. Additional rf cavities are presently in the construction stage. With the presently installed rf power amplifiers and a complement of four rf cavities, a beam energy of 3 GeV, with a 300-mA circulating beam, can be achieved.

There is a growing consensus that, in the coming years, a high-energy ring, operating at an energy on the order of 6 GeV, will become increasingly attractive for a variety of experiments. Thus, the Booster II synchrotron will not only be capable of injecting into the energy-upgraded XRAY ring, at an energy of 3 GeV, but it will also be designed to accelerate electrons to 6 GeV for full-energy injection into the high-energy "undulator/wiggler" storage ring to be constructed in the second stage of the program.

FACILITIES (USA)

The basic parameters of Booster II are as follows:

Energy	6	GeV
Circumference	340.3	meters
Magnetic radius	26.7	meters
Beam current	5	mA
Radio frequency	370.2	MHz

Because the initial operating energy will be only 3 GeV, construction of a good fraction of the rf hardware could be postponed. It is desired, however, to avoid subsequent interruptions of the XRAY program; therefore, the full rf-cavity complement will be installed during the first stage of the construction program.

The siting and construction of Booster II and its associated tunnels and service buildings would have to take into account the subsequent construction of the 6-GeV undulator/wiggler (U/W) ring, which would have to be carried out with no interruption of the XRAY-ring experimental program. Reinjection of the 3-GeV Booster II beam into the XRAY ring has been examined in a preliminary manner. In crossing the XRAY experimental area, the charged-particle beam transport would pass under a number of photon lines in a manner analogous to what is presently done with the transfer line from Booster I to the VUV storage ring. Table 11 provides cost estimates for the various components involved in the construction of Booster II.

In order to improve the present charge-transfer rates into the VUV and the XRAY rings (and, from a longer-range point of view, into the U/W ring), an improvement program to increase the prebunch intensity in Booster I is being carried out. This program involves not only incorporation of a new state-of-the-art gridded electron gun but also the rebunching, at 800 MeV, of five bunches into one bunch, by means of a new 10.6-MHz rf unit. As a result, significantly shortened charging times will be achievable in the two existing storage rings, and, after completion of the U/W ring, charging of the three rings from zero circulating beam to design current values would be done in significantly less than 30 minutes.

A preliminary study of the high-electron-energy U/W storage ring has been carried out with the objective of potentially providing for ultimate-brightness radiation sources in the hard part of the x-ray spectrum. The design parameters were guided toward the use of a 0.86-Å first-order spectral peak from a state-of-the-art permanent-magnet undulator source. These considerations led to a maximum electron energy of 6 GeV. While still keeping economic factors in sight, the design of this storage ring was optimized for minimum source emittance, thus resulting in the principle parameters shown in Table 12.

With its superperiodicity of 16, this ring would permit the ultimate use of $(28-N_w)$ undulators, N_w wiggler sources, $(32-N_{ws})$ dipole sources, and N_{ws} short wiggler sources. Table 13 gives more detail on these potential sources and compares them with those of the "P-ESRF," the European Synchrotron Radiation Facility, which is proposed for construction at a cost of approximately \$150 million.

Table 11

Cost Estimates for the Construction of Booster II: NLS Phase III
(In FY85 Millions of Dollars)

A. Engineering, Design, and Inspection	5.50
B. Booster II	
1. Principal Systems	14.76
2. Associated Equipment	1.48
C. Conventional Construction	4.87
	Subtotal 26.61
D. Contingency at 20%	5.32
	TOTAL 31.93

Table 12

NLS High-Energy U/W Ring
Preliminary Parameters

Energy (GeV)	6
Periodicity	16
Circumference (meters)	753.58
Bending Radius (meters)	33.40
v_H, v_y	-25, -9
Momentum Compaction, α_P	4.5×10^{-4}
ϵ_H (m·rad)	0.7×10^{-8}
ϵ_V (m·rad)	7×10^{-10}
Dipole Field, B(kG)	7.5
Sextupole strength, B'' (kG/m ²)	-120
Number of "High Beta" long straights ($X_p=0$)	16
Number of "Low Beta" long straights ($X_p=0$)	16
Beam Current (mA)	250
Bunch Length (at I=0) (ps)	22

Table 13

A Comparison Between the NSLS U/W Ring and the ESRF

<u>Ports and Stations</u>	<u>U/W Ring</u>	<u>P-ESRF</u>
A. BENDING MAGNETS		
λ_c (A)	0.86	2
Flux at λ_c /mrad (photons/mrad/1% BW)	2.3×10^{13}	2.7×10^{13}
Number of Ports	$< (32 - N_{ws})$	10
mrad/port	10	10
B. MULTIPOLE WIGGLERS		
λ_c (A)	0.35	1
Flux at λ_c /mrad (photons/mrad/1% BW)	2.2×10^{15}	3.2×10^{14}
Number of Ports	N_w	38
mrad/port	2	2 (:2)
C. SHORT WIGGLERS		
λ_c (A)	0.09 to 0.35	0.25
Flux at λ_c /mrad (photons/mrad/1% BW)	8.8×10^{14}	2.7×10^{13}
Number of Ports	$< N_{ws}$	10
mrad/port	2	12 (:3)
D. UNDULATORS		
λ_1 (A)	0.86	
Number of Ports	$< (28 - N_w)$	

Stanford University, SSRL--6-GeV-Ring Facility

SSRL has been studying new ring designs that are optimized around wiggler/undulator sources that give orders-of-magnitude-greater flux and brightness than bending magnets. SSRL experience with high-power wigglers reinforces the belief that, because of thermal problems, we are close to the limit of x-ray intensities that can be used at existing rings and that major advances in x-ray intensities and brightness require x-ray undulators that concentrate the spectrum in the desired region.

To utilize x-ray undulators effectively, high-energy storage rings (5 to 6 GeV) with very low emittance are required, along with a large number of straight sections for insertion devices. In the effort to achieve additional capabilities in the soft x-ray/VUV region, SSRL has studied the concept of having a 2-GeV ring with very long straight sections in the same housing as a 6-GeV ring. The rings would share the facility, thus reducing costs, and beamlines from each ring would alternate (spaced at six degrees) around the circumference.

Various designs for such a dual-ring system have been studied. A proposal and a conceptual design report for a 6-GeV facility are expected during 1984. The parameters now being considered are shown in Table 14.

Table 14

SSRL 6-GeV-Ring Parameters

Energy (GeV)	6
Circumference (meters)	532
Beam Emittance (m·rad)	5.7×10^{-9}
Beam Current	
per bunch (mA)	< 5.0
total (mA)	< 100
Beam Lifetime	
Touschek (h)	20
Coulomb Scattering (h)	20
Gas Bremstrahlung (h)	20
Total (h)	6.7
Bunch Length (ps)	~100
Average Vacuum (torr)	5.10^{-9}
SR Power (kW)	600
Insertions	
High Brightness	10
free length L(meters)	4
Small Spot Size	20
free length L(meters)	2

Some of the major design criteria beyond the need for a 6-GeV ring are:

- The beam current--both per bunch and total--should be moderate.
- The design should aim for the smallest reasonable beam emittance.
- In some insertions the brightness of the photon beams from an undulator should be maximized. This is achieved by reducing the beam divergence to such a level that the spectral line width as determined by the divergence is equivalent to the line width due to a 100-period undulator.
- There should be space for 30 insertion devices in the ring, and the aperture requirements for the beams should be minimized in both planes to allow short-period insertion devices to deflect the beam in either plane.
- The beam lifetime should be at least 10 hours.

These criteria are met with a new magnet-lattice arrangement using "triplett achromats" in between straight sections. This arrangement provides a small emittance and good flexibility and reduces the circumference of the ring by 30% for a given number of straight sections.

The radiation characteristics of the many possible sources in this ring are shown in Table 15.

Radiation Characteristics of Possible SSRL 6-GeV-Ring Sources

High-Brightness Insertions

Energy (GeV)	6
Beam Size σ_x/σ_y (μm)	324/116
Beam Divergence α_x'/α_y' (μrad)	13/13
Line width/ γ (100 periods)	8.5×10^{-6}
Total Line Width/ γ	2.0×10^{-5}
Minimum Gap G_x/G_y (mm)	7/5.5
Highest Fund Photon Energy ϵ_{ph} (keV)	20

Small-Spot-Size Insertions

Energy (GeV)	6
Beam Size $\sigma_x\sigma_y$ (μm)	48/41
Beam Divergence α_x'/α_y' (μrad)	48/41
Minimum Gap G_x/G_y (mm)	2/2
Critical Photon Energy $B_W = 20 \text{ kB } \epsilon_c$ (keV)	47.5

Bending Magnets

Energy (GeV)	6
Bend Field (kG)	10.5
Critical Photon Energy (keV)	25

As in any high-energy ring with undulators and wigglers, a major design issue is handling the photon-beam power on downstream components in the beamline. The latest beamline at SPEAR (LBL/Exxon/SSRL 54-pole, 1.2-T wiggler) has front-end components designed to take power densities of 200 W/mm^2 . Present downstream optical elements can take considerably less power density and many possible solutions are being considered. They include in-vacuum monochromators, new materials including multilayer and SiC mirrors, and 100-meter-long beamlines. With the assumption that power densities should not exceed twice the present level (i.e., $< 400 \text{ W/mm}^2$), SSRL has studied a wide range of undulator/wiggler parameters and has concluded that:

- An array of undulators can cover the energy range of from 3 to 21 keV in the fundamental, with conservative gaps and a source brightness of 10^{18} to 10^{19} photons/sec $\text{mrad}^2 \cdot 0.1\text{A} \cdot 0.1\% \text{BW}$.
- Given the parameters of the 6-GeV ring, wigglers can operate with critical energies up to 40 keV.
- Continued research and development is required to improve the downstream optical components; much experience will be gained from the present high-power lines on SPEAR.

Summary of Future Facilities

It is clear from the above that future SR facilities will predominately use insertion devices and, as a result, will achieve source brightness that is orders of magnitude higher than would otherwise be possible. The storage-ring designs reflect this design direction in having small beam emittance and many insertions whose beam optics are tailored for undulators and wigglers. These trends are illustrated in Table 16, which gives a summary comparison of machine parameters and source characteristics for some representative existing and proposed SR facilities.

The ALS has been formally proposed for construction, and its projected performance and cost have been detailed above. This facility would enhance the US capability in the VUV and soft x-ray energy range.

In the harder x-ray range, there are several studies in progress, and proposals for construction are currently being initiated. These facilities will again use insertion-device-based storage rings but will operate at higher energies--around 5 to 6 GeV. Because injection at the operating energy is becoming increasingly important in optimizing the storage-ring design and in improving operation, it is worth noting that there are three locations in the USA where existing electron accelerators could be used as injectors, thereby reducing the construction cost of a high-energy facility. At Cornell studies have begun on a possible dedicated synchrotron light source that could use the high-energy-electron synchrotron as an injector. The cost of a 5 to 6-GeV facility including an injector is estimated to be approximately \$168 million in FY85 dollars. This figure includes the experimental areas and an initial complement of approximately 10 undulator/wiggler beamlines. The designs could eventually accommodate 30 or more

Table 16

Storage-Ring and Device Parameters for Representative Facilities

	NSLS			SSRL		
	SPEAR (achieved)	VUV (achieved)	X-ray (design)	ALS (design)	PEP (design)	SSRL--6-GeV (design)
STORAGE RING						
Energy (GeV)	3	0.75	25	1.3 (1.9 max.)	15	6
Total current (mA)	100	300	500	400	20	100
Number of bunches	16	1	1 to 30	250	3	20 to 30
2 σ bunch length (ps)	~ 200	400	330	23	70	200
Circumference (m)	234	50	170	182.4	2200	532
Horizontal						
Emittance (π -mrad)	4.5×10^{-7}	1×10^{-7}	1×10^{-7}	6.8×10^{-9}	1.2×10^{-7}	4.6×10^{-9}
Injection energy (GeV)	2.5	600 MeV	700 MeV	1.3	15	6
Number of bends	36	8	16	24	192	90
Number of quads	52	20	56	84	230	180
Number of straight sections for insertion devices	15	2	6	12	1*	30
Length of straight sections for insertion devices (m)	13 - 12m 2 - 5m	2.5	4.5	6	2*	10 - 4.3m (for undulators) 20 - 2.3m (for wigglers)
Beam lifetime (h)	15	1.5	8	8	8	6.7

TABLE CONTINUED ON NEXT PAGE

Table 16 (Continued)

Storage-Ring and Device Parameters for Representative Facilities

	NSLS			ALS (design)	SSRL	
	SPEAR (achieved)	VUV (achieved)	X-ray (design)		PEP (design)	SSRL--6-GeV (design)
PHOTON BEAMS						
--Bends						
Critical energy E_C (eV)	4700	430	5000	1230	$4.5 \times 10^4 \dagger$	2.5×10^4
Photon flux at E_C for all ϕ (photons/s.mrad $\theta=0.1\%$ BW)	4.8×10^{12}	3×10^{12}	2×10^{13}	8.3×10^{12}	$4.8 \times 10^{12} \dagger$	9.6×10^{12}
--Wiggler						
Peak magnetic field (kG)	18	NR \ddagger	20	20	NR	8
Number of poles	8	NR	11	80	NR	20
Critical energy E_C (eV)	10,800	NR	8000	2250	NR	19,200
Photon flux at E_C for all ϕ (photons/s.mrad $\theta=0.1\%$ BW)	3.8×10^{13}	NR	2×10^{14}	6.7×10^{14}	NR	1.9×10^{14}
Total beam power (W)	3690	NR	8600	8560	NR	2900
Beam power density at 10 m (W/cm 2)	500	NR	5600	991	NR	8600 \S
--Undulator						
K factor	1	1	1	1	1	1
Full magnet gap (cm)	~ 3.5	1	0.7	1.2	5.8	0.8
Period length (cm)	6.1	2.6	2	2.67	7.5	2.06
Number of periods	30	96	150	187	26	200
First harmonic energy E_1 (eV)	950	-	-	401	19,000	11,000
Spectral brilliance at E_1 (photons/s.mm 2 .mrad 2 .0.1% BW)	2×10^{15}	1×10^{17}	2×10^{17}	5×10^{18}	$\sim 9 \times 10^{14}$	3×10^{19}
Total beam power (W)	35	50	1700	344	115	2460
Beam power density at 10m (W/cm 2)	~ 600	110	4.1×10^4	930	1245	1.35×10^5
Beam power in central spot (W)	NR	0.7	800	9.3	NR	46

*One 2-m-long undulator is now in development for PEP. Future undulators could be 4 to 5-m long.

\dagger Achieved

\ddagger NR = not relevant

\S Front-end components would be located 25 m or more away from the source; power density drops quadratically with the distance from the source.

independently optimized beamlines. This estimate is comparable to that for the ESRF, which is in an advanced design stage.

In addition to the construction of new dedicated facilities, plans are underway to explore the physics opportunities of hard x-rays from undulators on existing high-energy storage rings such as PEP and CHESS. This effort raises the question of whether these facilities could be expanded as an alternative to the construction of a new ring. These storage rings were designed for colliding electron/positron beams, and their use for high-energy physics is expected to continue for many years. Parasitic or semidedicated operation of these rings for SR use is possible, but this would put severe technical limitations on the number and quality of insertion-device-based beamlines that could be made available. Even if one of these storage rings were to become available for dedicated SR use, their large beam emittance, their lack of provisions for installing insertions, and their location deep underground would make them a poor technical and economic choice as a basis for an advanced SR facility.

Cost Projections For Synchrotron-Facilities Development

Introduction

The committee had as its primary objective the establishment of priorities for the development of SR facilities in this country over the next decade. This development is to proceed through the utilization of the current generation of new machine, through the development of existing straight sections by means of insertion devices, and through the building of new, insertion-device-based machines.

The current generation of "new" synchrotron facility offers both increased brightness, due to better machine design, and added capability, due

to the expanded number of beamlines. There are also limited opportunities to develop and utilize insertion devices. The primary impact of this current generation of machine will be to:

- 1) make available a 10^2 to 10^4 increase in brightness, compared to previous machines, and
- 2) allow access by a wider community to the benefits of SR.

The increased beam quality achieved by these machines and the greater beam time they offer will allow expansion of ongoing studies and will cross the threshold for studies that were previously unfeasible. Intensified efforts at making these facilities "user friendly" will increase involvement by the materials-science and technology communities. Important research and development on beamline and endstation performance will be conducted to provide relatively low-cost gains in overall performance.

The development of insertion-device opportunities on existing machines will begin to establish the science possible with those devices and the technology applicable to the next-generation machine. Given the rapid movement in technology in this area, it is anticipated that there will be further advances over the near term. The revolutionary capabilities of these devices is expected to draw to the synchrotron area new communities of scientists and materials technologists, which will establish a new driving force for further capacity and expanded capability.

The construction of insertion-device-based machines, if implemented on the most expeditious schedule technically possible, cannot be expected to greatly impact the field until the late 1980s or early 1990s at best. The demand will then be high for insertion-device capability, as the emphasis is shifted to techniques requiring insertion-device performance.

Facility Cost Projections

There are three primary components to the facilities-development picture over the next 10 years: development of insertion-device capability on existing machines, design and construction of a high-energy facility to produce undulator radiation in the hard x-ray region, and construction of a low-energy facility to provide undulator capability in the soft x-ray ultraviolet (XUV) region. The individual development schedules for these components are as follows:

Development of Existing Straight Sections for Insertions -- There currently exists the following potential for new insertion-device development at dedicated facilities:

FACILITIES (USA)

<u>Facility</u>	<u>Number of Straight Sections</u>	<u>Approximate Development Cost per Beamline (FY85 Millions of Dollars)</u>
SSRL	4(short term) ^a 4(fully dedicated)	2.0 to 4.0
NSLS	7 ^b	0.8 to 1.4
SRC	4	1.5

^aOne of these is included in SEPPF.

^bSix are included for development in Phase II.

The actual development costs will of course depend to a great deal on the complexity of the beamlines involved. Their development should proceed at a measured pace to take advantage of technological advances, but at the same time user demand will force rapid development of a basic capacity.

The High-Energy Facility -- The high-energy facility is in the conceptual development stage. The design and engineering work needed to get to the proposal stage will take approximately two years. The construction-and-procurement phase will require approximately five years and has a projected cost of \$168 million (in FY85 dollars), which can be broken down as follows:

Approximate Cost Breakdown for a 6-GeV Facility ^a
(In FY85 Millions of Dollars)

Engineering Design and Inspection	17
Conventional Construction	40
Technical Construction and Capital Equipment ^b	83
Contingency	<u>28</u>
TOTAL	168

^aCost figures provided by SSRL--figures are not reviewed

^bIncludes 10 instrumented beamlines and \$14 million for an injector

The Low-Energy Facility -- The low-energy facility can be constructed from the existing ALS design at a cost of \$72.6 million (in FY85 dollars). Construction will require four years. The cost is broken down as follows:

ALS Construction Costs
(In FY85 Millions of Dollars)

Accelerator Systems	30.5
Beamline Systems ^a	30.4
Conventional Facilities	<u>11.7</u>
TOTAL	72.6

^aIncludes 14 branch lines on 6 insertion-device ports

Users

Overview

The report on the "Current Status of Facilities Dedicated to the Production of Synchrotron Radiation" (the Lynch Report), published in 1983, concluded that user demand would saturate capacity by 1985. While the primary motivation for the actions recommended in this report is the creation of new opportunities in science and technology rather than the creation of added capacity, we found that indeed the Lynch Report projections seem to be valid. The NSLS XUV-ring bending-magnet ports are fully subscribed, and no more than four ports remain open on the XR ring. The SRC is approximately 70% committed even before becoming operational, and SSRL remains heavily oversubscribed. Development of the available straight sections by means of insertion devices is, of course, high among our recommendations, in concurrence with the Lynch report.

The following table shows, for the indicated years, the user count at various SR facilities and the number of publications arising from work done at each facility. The user count shown is the number of scientists who actually came to the facility to take data. Others associated with the proposals but not directly involved in data collection are not included. The user counts from 1983 are high in that they include the members of the NSLS x-ray PRTs who would have been at the facility had it been operational. NOTE: There is some overlap of users between the various facilities, in particular between NSLS and SSRL but between the others as well. This overlap is not accounted for in any manner.

	<u>Users</u>			<u>Publications</u>		
	<u>1981</u>	<u>1982</u>	<u>1983</u>	<u>1981</u>	<u>1982</u>	<u>1983</u>
SSRL	167	249	275	136	168	162
SRC	135	130	96	78	84	78
NSLS	-	-	398 ^a	-	-	40
SURF	57	39	39	30	42	20
CHESS	<u>15^b</u>	<u>186</u>	<u>249</u>	<u>4</u>	<u>30</u>	<u>36^c</u>
TOTALS	374	604	1057	248	324	336

^aIncludes x-ray PRT members who would have been using the facility if it had been operating; 124 users actually took data on the VUV ring.

^bOperation started in December 1981.

^c70 more publications are presently in print.

FACILITIES (USA)

A general idea of the SR-demand distribution across disciplinary boundaries can be obtained from the current breakdown of SSRL proposals, which is as follows:

Physical sciences	35%
Materials sciences	28%
Biology and medicine	21%
Chemical sciences	16%

User Interactions

SR facilities interact with a large number of users having various levels of expertise, under a variety of sometimes difficult circumstances. In order that efficient use be made of these limited and unique facilities, it is imperative that user interactions be carefully thought out and that facility personnel and users clearly understand their responsibilities and prerogatives. The classes of people involved in these interactions include facility managers, facility research personnel, facility technical personnel, scientific personnel from research groups that have built beamlines, users who have had extensive SR experience, and users who have had little or no SR experience. Furthermore, the users may need to operate under a variety of constraints ranging from the open research characteristic of university groups, to proprietary research having commercial restrictions, and to defense research requiring classification restrictions. The range of sociological interactions is large and complex. It takes effort and goodwill to assure that these facilities operate efficiently.

Dedicated SR sources operate 16 to 24 hours per day, seven days per week, for a large part of the year. The time scheduled for each user is highly variable, depending on the experimental requirements, and it is possible to have several user groups alternate in the use of a beamline during a day. Large research groups may have the manpower to operate for the required long hours, but small user groups and individuals require assistance. Such assistance might consist of cooperative interactions between small groups having common interests or interactions between the small user and a larger group. Cooperative research might also involve the user group and facility professionals, or the user group may arrange assistance from SR-facility technical personnel.

The SR-facility staff has responsibility for development of new instrumentation for the facility. Qualified user groups can greatly assist in this task. In fact, much of the advanced instrumentation at Tantalus, at SSRL, and at NSLS has been developed by user groups. Unfortunately, as facilities become larger and more complicated, sheer cost may prevent highly qualified university-based groups from developing beamlines. To assure continued participation by such groups, we urge that a sizable fraction (say 75%) of the beamlines at new facilities be developed by means of collaborations between such university groups and the facility staff. These collaborations would be similar to PRTs but with the important difference that funding would be provided by the instrumentation budget of the facility. Groups participating would be selected by a peer-review process to ensure their capability and suitability for the development proposed.

The policies that govern the use of beamlines will be developed by each facility to suit the local needs and conditions. In general, beamlines developed by the SR facility and by PRTs should be available to the general user community for a significant percent of the operating time. Beamlines developed by SR user groups other than PRTs should also be available to the general community for a part of the time. Even in the case in which a company develops a beamline at its own expense and pays "full cost" for the use of the beamline, use by the external community should be allowed and arranged through the SR-facility management. An exception to this cooperative-use arrangement may arise in the case of beamlines that are funded by the defense laboratories for classified work, but even in this case time should be available, given suitable controls.

The SR-facility management has the obligation to provide access on a "user friendly" basis. This obligation entails many things such as: adequate documentation of the facility equipment, along with assistance or instruction in developing the expertise to use it properly; adequate documentation for the required computer programs; controlled access to at least a limited range of support facilities and services such as storerooms, shops, office help, and darkrooms; and possibly other forms of assistance. While these forms vary, each SR-facility management has the obligation to facilitate the use of the beamlines. The "friendliness" of facilities is determined, in large part, by the helpfulness and cordiality of the staff with whom the users interact. It is exceedingly important, therefore, that such people be selected not only for their scientific or technical competence but also for their willingness to serve the user community. These qualities will be especially important in attracting future users from areas such as medicine and materials science. In general a "user committee" should exist to act as an intermediary between the user and the facility management when necessary. In addition to the above forms of assistance, it should be possible for the SR facility to help provide for housing and other amenities as deemed appropriate.

Scheduling of time on beamlines is a difficult and sensitive matter because the demand for usage is expected to exceed the available time. Again, only guidelines can be set down in view of the variety of beamlines and users. Scheduling procedures should be reviewed by the user committee. Proposals in the basic-science, applied-science, and technology categories should be judged on the basis of suitable standards in each category, and a balance should be sought between the three groups.

Research and Development

In order to develop the next-generation x-ray synchrotron facilities, a coherent long-range R&D plan must be implemented. The new SR facilities will be designed to incorporate a large number of undulators, which will provide for extreme-brightness, tunable radiation sources well into the hard x-ray region (15 to 20 keV), and wigglers, which will provide for photon energies into the 100-keV region. Such facilities will entail new problems in accelerator physics, in the development of undulator and wiggler sources, and in the handling of orders-of-magnitude-higher photon fluxes on beamline components such as monochromator crystals and grazing-incidence mirrors and gratings.

FACILITIES (USA)

An overall plan, therefore, must address the following topics: (1) the development of science-driven goals for the performance of the machine, the insertion devices, and the beamline instrumentation, and (2) the implementation of appropriate R&D to assure successful achievement of these goals. Each of these topics is discussed below.

Development of Science-Driven Goals

This process is the scientific core of the development of SR facilities. It is by nature an evolutionary, community-wide process that is continually underway. We recommend that this process be fostered by the Department of Energy (DOE) sponsorship of periodic workshops to be held alternately at various laboratories. These workshops should be organized by a local committee of the host laboratory, working together with a national advisory group; the workshops should be international in scope. Travel budgets should be provided to encourage the attendance of the most experienced people and of those students and postdocs who are without adequate financial resources.

Indeed, one workshop has already been held at SSRL in June 1983, and another is planned for the summer of 1984. These workshops are endorsed by this committee provided that they involve international participation and that it is understood that the site chosen for such workshops will vary in the future. It is to the great benefit of the synchrotron community to encourage the participation of as many institutions as possible in the planning for next-generation sources. Further, it is our hope that a number of institutions will ultimately make proposals to construct the planned facility.

R&D Activities

Unlike the development of science-driven goals, the actual new-ring R&D activities pursued at each of the various institutions involved must be integrated with that institution's other R&D activities and must be commensurate with the talents and interests of the staff scientists at the institution. Such a process will necessarily involve some duplication of effort, but such duplication serves an essential function in scientific research and should not be considered wasteful. Both NSLS and SSRL have moved rapidly to develop R&D plans for FY 85 and FY 86 at the approximate level of \$1.25M/year at each institution. We strongly recommend funding of these programs. The following summarizes the items that are considered important to address in these R&D plans; many of these items appear in the plans already developed.

Machine-Physics R&D

1. Multibunch instabilities
2. Ion trapping, measurements and calculations; the feasibility of the use of positron rings to alleviate ion trapping
3. Beam steering, orbit stability
4. Full-energy injection; utilization of a top-off mode to achieve "steady-state" operation

5. Vacuum studies (the vacuum is more important in low-emittance machines); desorption studies
6. Ring-lattice-structure studies, modular-prototype development
7. Development of new injector technology
8. New ring-control systems and beam diagnostics
9. Time-structure studies
10. Coupling of horizontal to vertical emittance.

Insertion-Device R&D

1. Calculation of photon fields from wigglers and undulators
2. Use of higher undulator harmonics
3. Minimum gap requirements
4. New methods of producing periodic magnet fields (e.g., the use of microwave devices)
5. Helical wigglers and other circularly polarizing devices
6. Permanent-magnet/hybrid-structure R&D, optimization studies, and in-vacuum devices
7. PEP undulators

Beamline-Instrumentation R&D

1. Beam-steering systems, detectors
2. Beryllium-window R&D, determination of thermal-stress limits
3. Thermal tolerances for optical elements; tests with simulated heating by lasers and electron beams
4. Mirror surfaces and effects of radiation, roughness, coatings, and metrology
5. Multilayer optics; focusing and monochromatizing
6. Ray tracing under thermally stressed conditions
7. Absolute-flux monitors
8. Optical observations of source image
9. Tests of cooling schemes (e.g., radiative cooling)

FACILITIES (USA)

10. Development of refractory x-ray optical elements, notably crystals for monochromators
11. Study of superficial contamination and desorption due to intense x-ray beams

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APPENDIX A

November 14, 1983 Letter to the Department of Energy

November 14, 1983

Dr. Alvin W. Trivelpiece
Director, Office of Energy Research
Department of Energy
Washington, D.C. 20585

Dear Al:

In this letter we will respond to your request to provide a status report on the Committee's deliberations on a long-range plan for advanced synchrotron radiation (SR) facilities in the U.S. We have met with over 75 scientists in Albuquerque on October 8 and 9, 1983, and in executive session at Stanford on October 26, 1983, and in Boston for two days on November 12 and 13, 1983. In this series of meetings we performed a critical review of both the scientific imperatives and facility options. We do not expect a final report until February 15, 1984. The great breadth and diversity of both the scientific and technological impact and facility options are the strength of SR. It is, therefore, a significant task to make sure all the opportunities and problems are correctly presented and documented in our final report. However, we can, at this time, provide you with an overview of the situation and a prioritized list of recommendations which we are certain will be featured in our final report.

OVERVIEW

The scientific and technological impact of synchrotron-based research is growing rapidly with numerous high quality advances in chemistry, biology, and physics, as well as in medical and materials technologies. As exciting as the past has been, the future opportunities in both science and technology are even greater. The new sources just being commissioned already offer a significant gain in capability from which new science will evolve. Insertion devices, which will form the basis of a revolutionary new generation of machines, promise such enormous gains in radiation flux and brightness that fundamentally new science can be approached.

There are significant plans already underway in Japan and Europe to exploit the new opportunities presented by insertion devices. Given the long lead time to develop these facilities, this country needs an aggressive program to provide such capabilities to our scientific and technological communities. The following recommendations represent such a program which we believe is justified by the scientific promise and practical importance of synchrotron radiation research.

RECOMMENDATIONS FOR A TEN-YEAR PLAN FOR SYNCHROTRON RADIATION FACILITIES AND SPECIFIC RECOMMENDATIONS FOR THE FY85 BUDGET CYCLE

The Committee recommends as its top priority that steps be taken to assure the timely completion of commissioning of NSLS and SRC as well as providing adequate operations budgets to assure the effective utilization of all existing facilities.

The future of synchrotron radiation research is clearly dependent on the significant gains offered by insertion devices. Our unanimous prioritized recommendations to exploit these new opportunities are as follows:

- 1) To realize the full potential of existing facilities, the Committee recommends expeditious completion of current projects to construct insertion device beamlines at SRC, NSLS and SSRL.
- 2) The Committee recommends the construction of a 6 GeV storage ring beginning in 1987 as a dedicated national facility. To achieve this objective, appropriate R&D funds must be allocated in FY85 and FY86.
- 3) The Committee recommends proceeding with the ALS in FY85 as a dedicated national facility.

The Committee strongly recommends that no action on a lower priority recommendation interfere with the timely pursuit of the higher priority items.

COMMENTS

The Committee determined that the physics of synchrotron radiation and insertion devices dictates different energy machines for the x-ray and XUV regions of the spectrum. The Committee unanimously concluded that if only a single new facility was to become available, the 6 GeV facility must have priority because it addresses regions of the spectrum and new science not accessible with insertion devices on existing dedicated facilities. In such an eventuality, the existing lower energy machines could be used to expand XUV insertion-based capability.

The difficulties presently being experienced in the commissioning of the newly constructed machines are not fundamental in nature and result partially from over-zealous attempts at economy. Therefore, our recommendations reflect the need for adequate funding for their commissioning and operations.

In our meetings and deliberations we received strong support for synchrotron radiation research from a broad spectrum of the scientific, industrial, and defense interests. We heard of achieved and potential breakthroughs in many areas, including catalysis, protein crystallography, angiography, plasma physics, and a broad spectrum of materials science.

There will clearly be considerable future growth in industrial participation as long as their participation is facilitated by user friendly instrumentation and the protection of their proprietary interests. The Committee also concluded that university participation would be greatly augmented if the funding for new beamlines at future and existing facilities was provided in such a way that outside groups can participate; and the facilities would profit greatly from their expertise. A proposal-based, peer reviewed approach for selection of outside participants is strongly recommended.

The rapid developments in synchrotron radiation led the Committee to unanimously recommend that a group such as ours be convened on not less than a yearly basis to review current developments in the entire field and to make recommendations for future actions.

While the Committee has considerable work still to do before completing its final report, we can already conclude that the aggressive program in synchrotron radiation that we have recommended will contribute significantly to the scientific, technological, and defense strength of this country.

For the Committee,

P. Eisenberger

M. L. Knotek

ADVANCED SYNCHROTRON RADIATION RESEARCH PLANNING STUDY

Committee Members

Peter Eisenberger, Co-Chairman - Exxon
Michael L. Knotek, Co-Chairman - Sandia
Charles Fadley - U. of Hawaii
E. Ward Plumer - U. of Pennsylvania
Dave Moncton - Brookhaven National Lab
Farrel Lytle - Boeing
Fred Brown - U. of Illinois
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Keith Hodgson - Stanford U.
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Harry Gray - California Institute of Technology*
Dean Eastman - IBM
William Brinkman - Bell Labs
Guyford Stever - University Research Associates
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*Illness prevented attendance

APPENDIX B

**Survey of Synchrotron-Radiation Research Facilities
Outside the USA**

APPENDIX B

Survey of Synchrotron-Radiation Research Facilities Outside the USA

Introduction

Interest in synchrotron radiation (SR) research is growing so rapidly in many parts of the world that it is difficult to present an up-to-date comprehensive survey. This report attempts to briefly summarize the information that has been collected from numerous sources (questionnaires, laboratory reports, personal correspondence, etc.), with an emphasis on insertion devices and emittance, because these are of particular interest to the SR planning committee. The discussions of the different facilities vary greatly, reflecting the differences in the amount of information readily available.

In addition to providing a brief narrative about each facility (listed alphabetically by country), this appendix summarizes the available data in Table B-1 at the end of the appendix. More information, in the form of questionnaires filled out by individual laboratories, will be available in the proceedings of the 1983 U.S. National Conference on Synchrotron Radiation Instrumentation.

Also included at the end of this appendix are tabular summaries of European scientific interest (Table B-2) and of European storage-ring sources (Table B-3); these data are taken from the proceedings of the Scientific Workshop held at Stanford in July, 1983 and are also available in "Synchrotron Radiation Facilities in Europe" by B. Buras, Y. Farge and D. J. Thompson, ESRP-PG-1/83, March, 1983.

Additional information on SR facilities is contained in the Lynch Committee Report ("Current Status of Facilities Dedicated to the Production of Synchrotron Radiation," available from the Solid State Sciences Committee, 2101 Constitution Ave., Washington, D.C. 20418) and in A. Bienenstock and H. Winick, "Synchrotron Radiation Research--An Overview," Physics Today, 36:48-58, June 1983.

Brazil

Feasibility studies are in progress that may lead to a proposal for a dedicated light source in the 1 to 3-GeV range.

China

Two facilities are under construction in the People's Republic of China. Both are scheduled to begin operation in about 1988. One is HESYRL, an 800-MeV, fully dedicated light source being built at the University of Science and Technology in Hefei, Anhui. The ring design follows the very successful approach of BESSY; it will have four configurations (general purpose, high flux, high brightness, and short pulse) and 24 ports from bending magnets and 3 from insertions. The injector is a 200-MeV linac that is extendable to higher energy. About 160 scientists are planning research at the facility.

The other facility is a partly dedicated 2.8-GeV ring BEPC in Beijing that will primarily be used for colliding-beam studies. Initially, a small parasitic SR research program was envisioned here, using two bending-magnet ports and two wiggler ports. The ring has four wigglers to control beam size for colliding-beam studies. Recently the design group has been asked to start over again in its design for the ring in order to provide for a larger SR program. The new lattice will have four additional insertions for SR purposes. A 1.1 to 1.4-GeV e^+/e^- linac is the injector. About 200 scientists are planning SR research at this facility.

England

The Synchrotron Radiation Source (SRS), a 2.0-GeV dedicated ring and the world's first multi-GeV ring to be designed and built as a radiation source, has been in operation since 1980 in Daresbury, England. The injector is a 600-MeV synchrotron.

A major program is now underway to upgrade the SRS through the construction of new facilities. The status of this program is summarized in the comprehensive appendix to the Daresbury Annual Report 1982/83, compiled by A. Jackson and K. R. Lea and available from Daresbury. According to this report, there are 27 experimental stations in operation or in construction, 10 of which were operational at the end of the 82/83 year and 4 of which are not independently operable. There are 236 scientists involved with 75 active proposals, plus 96 additional scientists involved with 63 exploratory agreements (which receive small amounts of beam time). A 5-T, 3-pole superconducting wiggler has begun operation. The wide fan from this device will ultimately be shared by seven independently operable stations. A permanent-magnet undulator is in construction.

Because of the increasing appreciation of the importance of beam brightness, a proposal has been made to modify the SRS to reduce the horizontal emittance from the present value of 150 to 11×10^{-8} $\text{mm} \cdot \text{rad}$. This modification will require a 5-month shutdown projected to start in September 1985.

Europe

For several years scientists from many western-European countries have considered various designs for an optimized hard x-ray source to be called the European Synchrotron Radiation Facility (ESRF). Early in 1983 an important step was taken toward the realization of this proposal with the establishment of the European Synchrotron Radiation Project, tentatively located at CERN in Geneva, Switzerland. The main task of this project is to prepare a site-independent proposal for the ESRF, discussing the scientific case, machine design, and instrumentation. At present the planning is for a 5-GeV ring with a full-energy synchrotron injector. The ring would have very low emittance ($E_x = 7 \times 10^{-9}$ $\text{mm} \cdot \text{rad}$) and it would accommodate 32 wiggler/undulator insertions. Site proposals have been made for the facility by RISØ, Daresbury, Trieste, Strasbourg, and Dartmund; other site offers are expected. Progress is being made to secure the necessary multinational approvals, with authorization for construction expected by mid-1984.

France

In Orsay the LURE laboratory uses two operational rings and has one in construction. All rings use a 1.1-GeV e^+e^- linac for injection. The ACO 540-MeV ring is fully dedicated and has three bending-magnet ports serving 12 stations. Undulator/free-electron laser (FEL)/optical-klystron studies are pursued using one straight section. In 1983 the Orsay/Stanford group operated the first storage-ring FEL.

The DCI 1.72-GeV ring is used primarily for colliding-beam studies, with 25% of the beam time now dedicated to SR. In January, 1985 the DCI will become fully dedicated to SR. Two bending-magnet ports now serve 10 stations. An undulator and a superconducting wiggler are in construction. More than 350 scientists are involved with research at ACO and DCI and are planning research at Super-ACO.

Super-ACO, an 800-MeV dedicated source, is under construction and is scheduled for operation in late 1986. It will be a low-emittance ring ($E_x = 3.0 \times 10^{-8} \text{ m} \cdot \text{rad}$) with six straight sections for insertions. Twenty-four bending-magnet stations are also planned.

A study is in progress for a 240 to 500-MeV permanent-magnet storage ring. In collaboration with the Lawrence Berkeley Laboratory (LBL), a prototype dipole and quadrupole are being built.

Germany

The major facilities here are BESSY, an 800-MeV dedicated ring in Berlin, and HASYLAB, which utilizes the 5.5-GeV ring DORIS in Hamburg in both dedicated (30%) and parasitic modes. Both rings have full-energy injectors. In addition, there are two synchrotrons (0.5 and 2.5 GeV) in Bonn that are used for SR.

BESSY has 22 stations in operation on bending-magnet beamlines and 6 more in construction. A multipole wiggler and undulator are under construction. Part of the facility is devoted to soft x-ray lithography by industrial groups, part is devoted to radiometry by the PTB (Physikalisch-Technische Bundesanstalt), and the largest part is devoted to use by the general scientific community. Three different magnet optics have so far been implemented: x-ray, metro (which has the lowest emittance), and ISO (which has a bunch length of 25 ps). A bunch length of 10 ps should be possible in the future. The BESSY group is planning a compact synchrotron source (COSY). It will be a 560-MeV ring with 5-T superconducting bending magnets and a 38-cm radius of curvature. About 56 scientists are active in research at BESSY, excluding students and postdoctorates.

HASYLAB has 28 bending-magnet experimental stations in operation and more in construction. A multipole wiggler is being built. Four hundred scientists from more than 80 institutions are involved with SR research at HASYLAB, and there are others associated with the European Molecular Biology Laboratory outstation on DORIS. The annual HASYLAB Activity Reports contain much detailed information about the lab and its program.

India

The Indian government has approved in principal the construction of SR research facilities. Several design approaches are being considered.

Italy

The PULS project utilizes the ADONE 1.5-GeV ring in both dedicated and parasitic modes. Four bending-magnet stations, two wiggler stations, and one undulator station are in operation. More wiggler stations are under construction. Injection is from a linac at 300 MeV. About 200 scientists use the facility each year.

Japan

Four fully dedicated storage rings are now in operation, one dedicated ring is proposed, and two colliding-beam rings that will also be used for SR are under construction. In addition, a 1.3-GeV synchrotron is used for SR.

The main facility is the Photon Factory, a 2.5-GeV fully dedicated ring that has been in operation since 1982. Injection is at full energy from a linac. In operation are 19 experimental stations on bending-magnet lines, 4 on a superconducting wiggler line, and one on a permanent-magnet undulator line. The superconducting wiggler is unique in having a horizontal field and hence in producing a vertically polarized beam. The Photon Factory is located at the KEK Laboratory, which has two colliding-beam rings in progress. These rings will also be used parasitically for SR. The Accumulator ring (6 GeV) began operation in November, 1983, and the Tristan main ring (30 GeV) is under construction. Future plans include low-energy rings along the 2.5-GeV linac. Six hundred scientists are now involved in performing or planning research at the Photon Factory.

The TERAS 600-MeV dedicated ring has been in operation at the Electro-technical Laboratories in Tsukuba since 1982. It is used for lithography, radiometry, and other vacuum ultraviolet (VUV) studies. Injection is at 300 MeV from a linac.

The 380-MeV SOR ring at the Institute of Nuclear Science (INS) of the University of Tokyo is the first ring to be designed and built as a dedicated light source. Injection is at 300 MeV from the INS 1.3-GeV synchrotron. The storage ring began operation in 1974. The SOR ring program is under the direction of the Institute for Solid State Physics (ISSP) of the University of Tokyo. Five stations use bending-magnet radiation. A permanent-magnet undulator was tested in this ring, but limited experimental space precludes full utilization of such insertions. The ISSP group has proposed a new source, Super SOR, a 1.0-GeV low-emittance ring with eight long straight sections for insertions. This ring is described in the proceedings of the 1983 International Conference on High-Energy Accelerators (to be published).

At the Institute of Molecular Science in Okazaki, the first stored beam was obtained in November, 1983 in the 600-MeV UVSOR ring. Eleven experimental stations are under construction. The ring can accommodate four insertion devices. Injection is from a 600-MeV synchrotron. Two hundred scientists are planning research at this facility.

Sweden

The MAX 550-MeV storage ring/pulse stretcher is under construction at Lund. The facility will be shared by SR and nuclear-physics users. Four experimental stations are under construction.

Taiwan

The Taiwan Light Source (TLS), a 1-GeV low-emittance ring is approved for construction by the government and is now in design. Five straight sections will be available for insertions. It will be located near universities in an industrial park in Hsin Chu, about 50 miles from Taipei. About 100 Taiwanese scientists are planning to do research at the facility.

USSR

The main SR facilities here are at the Institute of Nuclear Physics in Novosibirsk, Siberia, which operates three storage rings, VEPP-2M, VEPP-3, and VEPP-4, all of which were built as colliding-beam rings. VEPP-2M is now largely used as a dedicated VUV/soft x-ray source, with eight experimental stations in use. This ring has an operational helical undulator originally built for high-energy-physics purposes but also useful as a source of circularly polarized radiation.

VEPP-3 supports a major program of x-ray research on its experimental stations. Much work has been done on VEPP-3 with insertion devices, including a 3.5-T, 20-pole superconducting wiggler and permanent-magnet undulators used primarily for optical-klystron experiments. Although VEPP-3 is not itself used for high-energy-physics experiments, it is part of the injection system for VEPP-4 and therefore only available for SR research for about 6 weeks per year.

VEPP-4 is a powerful x-ray source that is being fitted with beamlines, insertion devices, and experimental stations, of which some may already be in operation.

The Novosibirsk group has designed and built a 450-MeV storage ring that is being set up as a dedicated source at the Kurchatov Institute in Moscow. This ring will also be the injector to a proposed 2.5-GeV dedicated SR source.

A small 100-MeV storage ring, the N-100, has been operational at the Karkhov Physics Institute for many years.

Table B-1

STORAGE RING SOURCES OF SYNCHROTRON RADIATION

		H. WIWICK JANUARY 1984				
Location	Ring	Gev	Emittance (a) (10 ⁻⁶ p m-rad)	Exp. (b) Stations	Insertion (c) Devices	Status/ Use
<u>BRAZIL</u>						
<u>CHINA</u>						
Beijing	BEPC	2.8	66(18)		8	C/PDed
Hefei	HEPSYL	0.8	9(1.2)		3	C/Ded
<u>ENGLAND</u>						
Daresbury	SRS	2.0	150 (11)		1 (4)	Op/Ded
<u>EUROPE</u> (T.B.D.) (d)						
	ESRF	5	0.7		30	P/Ded
<u>FRANCE</u>						
Orsay	ACO	0.54	15	12	1	Op/Ded
	DCI	1.8	150	10	2 (2)	Op/PDed (e)
	Super ACO	0.8	3		6	C/Ded
<u>GERMANY</u>						
Hamburg	DORIS	3.7-5.5	27	30	1 (4)	Op/PDed
W. Berlin	BESSY	0.8	4(2)	28	1(2)	Op/Ded
	COSY	0.56	250	8	-	C/Ded
<u>INDIA</u>						
Poona		1.5				P/Ded
<u>ITALY</u>						
Frascati	ADONE	1.5	22.5	6	2(3-4)	Op/PDed
<u>JAPAN</u>						
Okasaki	UVSOR	0.6	8(3.3)	11	2(4)	Op/Ded
Tokyo	SOR	0.38	30	5	1	Op/Ded
	Super SOR	1.0	2.0		8	P/Ded
Tsukuba (KEK)	Photon Factory Accumulator	2.5	50(15)	24	2(7)	Op/Ded
	Tristan	6-8	48		3	C/Par
Tsukuba (ETL)	TERAS	0.6	18		0	C/Par
						Op/Ded
<u>SWEDEN</u>						
Lund	MAX	0.55	3	4	(2)	C/PDed
<u>TAIWAN</u>						
Hsin Chu	TLS	1.0	4		5	P/Ded
<u>U.S.A.</u>						
Berkeley	ALS	1.3	.68		12	P/Ded
Gaithersberg	SURF	0.28	27	11	-	Op/Ded
Ithaca	CESR	5.5	20(4)	6	1(3)	Op/Par
	New Ring	5-6				P/Ded
Stanford	SPEAR	3-4	45 (13)	19	4 (12)	Op/PDed
	PEP	15.0	15 (3)	1	1	C/Par
	SXRL	1.0	1.0		4	C/PDed
	New Ring	6.0	0.46		30	P/Ded
Stoughton	Tantalus	0.24	23	11	(2)	Op/Ded
	Aladdin	.75-1.0	(6.3)	19	(3)	Op/Ded
Upton	NSLS-I	0.75	13(9)	23	2	Op/Ded
	NSLS-II	2.5	(8)	32	4(5)	Op/Ded
	New Ring	6.0	0.7		32	P/Ded
<u>USSR</u>						
Karkhov	N-100	0.1				Op/Ded
Moscow	Kurchatov-I	0.45				C/Ded
	Kurchatov-II	2.5				P/Ded
Novosibirsk	VEPP-2M	0.7		8	2	Op/PDed
	VEPP-3	2.2		9	2	Op/PDed
	VEPP-4	5-7		6	2	Op/Par

(a) Emittance: For operational rings the lowest achieved horizontal emittance is given. When a range of operation energies is given the quoted emittance is at the lowest electron energy. Emittance scales as the square of electron energy. () indicates planned or possible future value. For rings not yet in operation the lowest design emittance is given.

(b) Experimental Stations: The total number of stations in operation or in construction in 1983 is given.

(c) Insertion Devices: For operational rings the number of insertion devices in use and in construction is given. () indicates maximum number possible. For rings not yet in operation the number given is the maximum possible number.

(d) T.B.D. - to be determined

(e) The DCI will be fully dedicated in January 1985.

F.S. = Feasibility study
Op = in operation

Ded = dedicated

P = Proposed
PDed = Partly dedicated

C = In construction
Par = parasitic

Table B-2

European Interest in Synchrotron Radiation Research (based on answers to a recent (1982) questionnaire)				
Number of groups (number of scientists)				
Country	Interested in S.R.	Have ex- perience in S.R.	Indicated problems	Made concrete proposals
Austria	7 (44)	3 (14)	3 (16)	3 (23)
Belgium	31 (214)	9 (71)	12 (112)	7 (62)
Denmark	14 (28)	3 (10)	3 (10)	3 (10)
Finland	11 (47)	6 (27)	5 (22)	4 (19)
France	145 (643)	89 (422)	93 (449)	77 (376)
Germany	82 (551)	53 (349)	41 (252)	26 (181)
Great Britain	57 (192)	43 (145)	33 (135)	26 (97)
Netherlands	2 (70)	1 (35)		
Norway	6 (27)	3 (8)		
Italy	83 (236)	54 (150)	26 (73)	19 (71)
Sweden	17 (86)	4 (16)	11 (54)	6 (29)
Total	455(2138)	268(1247)	227(1123)	171(868)

Table B-3

Storage Rings in Europe Emitting S.R.

Name Location	Electron GeV	Electron mA	Photon keV ϵ_c	Number of Stations	$W^x), U^x)$ FEL ^{x)}
ACO Orsay	0.54	150	0.31	15	U for FEL
MAX ⁺ Lund	0.55	(200) ⁺	0.31	0(3)	
BESSY Berlin	0.8	200 (500) ⁺	0.62	22	(W, FEL)
Super ACO [*] Orsay	0.8		0.65		(7U)
ADONE Frascati	1.5	≤ 100	1.5	4(5)	W, FEL
SRS Daresbury	2.0	280 (370) ⁺	3.2	8(27)	1W (1W)
DCI Orsay	1.8	300	3.4	7	(1-3W)
DORIS Hamburg	3.5- -5.6	30- -200	22.9	25	(1)
PETRA ** Hamburg	18.0	20	67.4	0	

x) See text; in parenthesis the number of devices under construction.

+) Expected values.

*) Under construction.

**) Not used for S.R. research

APPENDIX C

Alternate Photon Sources

APPENDIX C

Alternate Photon Sources

Laser Sources

Several groups have used nonlinear optical techniques to produce vacuum ultraviolet (VUV) and soft x-ray ultraviolet (XUV) pulses.¹ The shortest wavelength achieved to date, via seventh-harmonic generation in He gas, is 355 Å.² There has also recently been a report of a 930-Å stimulated emission in krypton gas.³ These experiments all require powerful pump lasers and complicated vacuum and gas-handling systems. Nevertheless, the equipment costs are modest compared to those of an ultraviolet (UV) synchrotron. Thus, it is pertinent to ask how laser UV sources might, in the future, compete with synchrotron UV sources.

Laser UV sources generally make use of high-order optical nonlinearities and require intense pump beams. They inevitably operate in a pulsed mode with relatively low repetition rate (10 Hz is typical). The average power generated by such devices is orders of magnitude lower than that of a UV synchrotron. Hence, for conventional, continuous-wave (CW) spectroscopy, the synchrotron will almost always be superior to a laser source. At present, most UV spectroscopy is CW spectroscopy.

Looking to the future, however, one can envisage a growing need for short, intense UV pulses. A number of biological and chemical-kinetics experiments require UV pulses in the nanosecond range; for other chemical applications and for many time-resolved condensed-matter-science measurements, picosecond pulses are needed.

The bunch structure of synchrotron beams naturally generates pulses in the 0.1 to 1.0-ns range, but it will be difficult to produce bunches shorter than 20 ps. Thus, direct picosecond spectroscopy with synchrotrons does not seem feasible. It has been suggested that picosecond time resolution might be achieved, in an indirect way, by making use of the extreme reproducibility (in shape and time) of the synchrotron pulses.⁴ That technique, termed Harmonic Phase-Shift Analysis, has recently been demonstrated at the picosecond level. Laser UV sources, on the other hand, often generate pulses in the picosecond range and could be modified, without excessive difficulty, to produce subpicosecond pulses with some degree of tunability. Thus, it can be argued that the laser source, rather than the synchrotron, is the natural tool for picosecond UV spectroscopy. A number of scientists hold that view, and several excellent groups in the U.S. are trying to develop pulsed UV sources for such purposes.

Until recently, laser sources for the XUV required complicated differential-pumping systems. The nonlinear process generating the radiation takes place in a moderately dense gas, whereas high vacuum is needed for subsequent experimentation. This difficulty has now been eliminated in systems employing pulsed supersonic jets. Though still inefficient, these devices promise ultimately to produce sufficient energy for such experiments as time-resolved XUV photoemission.

Facilities for generating XUV picosecond pulses via laser techniques will cost on the order of \$1M; though not inexpensive, the price is small compared to that of a synchrotron. At this stage, it is not clear that either laser sources or synchrotron sources can actually be used for picosecond UV spectroscopy. The current vigorous research effort on laser-produced XUV pulses should soon determine the potential of that technique. To date, there has not been a comparable experimental program concerning the use of synchrotron-generated UV pulses to achieve picosecond time resolution. Such measurements would be valuable; if successful, they would strengthen the case for constructing the Advanced Light Source (ALS). At present, however, the claim that ALS will be capable of doing subpicosecond UV spectroscopy is largely based on theoretical ideas that have not been extensively tested and that are viewed with some skepticism in the picosecond-optics community.

References -- Appendix C

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Plasma XUV Sources

Multimillion-degree plasmas emit intensely in the extreme UV and soft x-ray regions ($\lambda > 3 \text{ \AA}$). Hence, they are useful in the range below 1000 eV where operation of coherent direct-laser or harmonic-generation sources is not yet routine. Intensities available from plasma sources make them useful alternatives to synchrotron radiation (SR) for some experiments and superior to current storage-ring sources for other measurements.

Hot, dense laboratory plasmas of use as XUV sources are never large enough to be optically thick. That is, they are not blackbody radiators at short wavelengths. Their spectra consist of numerous lines on top of usually much weaker continua from recombination and Bremsstrahlung. At wavelengths longer than about 30 \AA , the lines can be so dense that plasma-emission spectra from high-atomic-number elements are effectively continua. Plasmas that are dense enough to emit x-rays intensely are commonly about 1 mm in extent. They produce x-radiation for times usually in the 100-ps to 100-ns range, depending on

the method of plasma heating. XUV radiation from plasmas is unpolarized, incoherent, and emitted into large solid angles ($>2\pi$ sr). Laboratory plasma XUV sources now typically cost \$200K to 400K.

Two types of energy sources are employed to produce x-ray hot plasmas-- lasers and electrical discharges.¹ Laser wavelengths in or near the 1 to 0.1- μ m range are of most interest. Nd systems (1.06 μ m, with harmonics at 0.53 and 0.35 μ m) and excimer lasers at 0.31 or 0.25 μ m have been or soon will be used for plasma XUV-source work. Capacitor banks, used either alone or with a pulse-forming network, are employed to produce electrical discharges greater than 100 kA that heat plasmas resistively or by magnetic-field-driven implosions. No matter how heated, plasma x-ray sources involve undesirable vapor (the expanding plasma) and sometimes debris. That is, they are not as clean as storage-ring sources.

X-rays from plasmas produced by very large, low-repetition-rate (10^{-3} Hz) Nd lasers have been widely measured in fusion-research programs for the past decade. Wavelengths as short as 0.1 A have been recorded. Now XUV radiation down to 1 A, produced by table-top Nd and excimer lasers that operate at 10 to 100 Hz, is being measured. Uses of soft x-ray emission from laser-heated plasmas are now increasing rapidly. The formation was announced recently of a U.S. company that will sell a lithography system using x-rays from laser-heated plasmas. Development of 100-W slab-glass Nd and excimer laser systems engineered for optimum production of x-ray-emitting plasmas is in progress. Such systems may be commercially available in a few years. Lasers for x-ray generation must have both high peak power (short energetic pulses), to achieve plasma temperatures adequate for efficient x-ray emission, and high average power (high repetition rate), to yield high average x-ray power.

Absorption of laser radiation by a target typically varies from about 50% with Nd at 1.06 μ m to over 75% for excimer-laser wavelengths near 0.25 μ m. As much as 30% of the incident laser energy can be emitted as XUV radiation in the 3 to 300-A region. Conversion efficiencies depend on target and focal conditions as well as on the laser-pulse characteristics. For some conditions, up to 0.1% of the incident laser energy can be re-emitted in a single strong x-ray line. XUV radiation from laser-heated plasmas mostly arises from a region less than 1 mm in diameter. In the 1 to 10-ns range, XUV pulse lengths are comparable to the laser pulse length. For picosecond lasers, plasma cooling extends x-ray emission times, so that x-ray pulses much shorter than 100 ps are uncommon. The limit on laser plasma x-ray emission times may be near 10 ps.

X-rays from large terawatt electrical-pulse generators have also been studied for the past ten years in fusion and weapons-related programs. Now, smaller, 10 to 100-MW pulsed-power systems are available commercially to produce x-ray-emitting plasmas at rates near 10^{-1} Hz. Their use is lagging the employment of lasers as plasma x-radiation sources because laser technology is more widely known and because laser systems tend to have more uses.

Materials for the plasmas in discharge-heated x-ray sources can originate from four different sources: 1) solid material (e.g., fine wires) placed across the interelectrode gap, 2) low-pressure gas filling the interelectrode region, 3) gas puffed into the cathode/anode gap immediately prior to the discharge, and 4) erosion of the electrodes. Of these, the puff sources are most reproducible, easiest to operate, and have the best chance of operation at rates exceeding

1 Hz. Whereas a laser-heated plasma will currently produce only 100 mJ of XUV radiation at 10 Hz (1 watt), commercial puff sources now yield about 20 joules at 10^{-1} Hz (2 watts). The line spectra from the puff source falls in the 4 to 40-A range, depending on the gas used, while x-radiation from CW laser plasmas tends to fall near 20 A. X-ray emission from discharge-heated plasmas is most intense from a cylindrical region about 1 mm in diameter and 1 cm long, with emission times of 10 to 100 ns.

Detailed comparisons of the radiation from plasma XUV sources with direct laser emission or SR are complex and can only be done on a case-by-case basis.² The wide variation in geometry among the different sources (e.g., emission directions) tends to require the use of different monochromators with different sources. However, in general, plasma sources of XUV radiation are superior to storage rings for peak power, and the opposite is true for average power. Some dynamic measurements, such as flash x-ray diffraction from or radiography of rapid events, require high peak intensities. Nonlinear x-ray-optics experiments that require high peak x-ray intensities are expected. Calibration of instrumentation for pulsed-x-ray measurements is also done with plasma radiation. Uses of laser plasma x-radiation in atomic, molecular, and solid state (surface) studies were examined recently, and many of them apply to discharge-heated sources also.³

In general, the development and use of plasma XUV sources is now where employments of SR sources was 10 to 15 years ago. Devices, especially lasers, that were engineered for other uses are being applied to x-ray generation, a process that is the equivalent of parasitic SR usage. However, lasers and discharge sources specifically designed for x-ray work are becoming increasingly available, and these items are analogous to dedicated storage rings. Plasma x-ray sources will not supplant storage rings. They may, however, be widely available for a variety of work within the next decade.

1. For recent review of plasma x-ray sources oriented toward x-ray lithography, see D. J. Nagel in N. G. Einspruch (Editor) VLSI Electronics, Volume 7, Plasma Processing for VLSI, Academic Press, New York (1984) p. 137.
2. E.-E. Kock (Editor) Handbook on Synchrotron Radiation, Vol. 1A, North-Holland, Amsterdam (1983) p. 41.
3. D. J. Nagel, "Characteristics and Uses of X-Radiation from Laser-Heated Plasmas," Society for Photographic Instrumentation, Vol. 447 (1984).

Free-Electron Laser (FEL) Sources

In the language of this report, the radiation provided by an FEL is stimulated undulator radiation. The first observation of FEL behavior was made in the early 1970s by Madey and coworkers on the Stanford superconducting linear accelerator. Since that time there has been a rush of activity. Using laboratory-scale accelerators (approximately 10 MeV), groups at Santa Barbara (funded by the Air Force) and at Bell Laboratories are exploring the use of FEL sources in the far infrared (75 μ m to 2 mm) region. Other groups, at

the National Synchrotron Light Source (NSLS) on the 750-MeV storage ring and in a joint Stanford/LURE project in France, have been pursuing FEL operation in the visible region, with the goal of ultimately moving into the UV and XUV regions. These storage-ring applications use insertion devices that are very similar to the ones described in this report but that have first harmonics in the visible region. The Stanford/LURE collaboration has successfully observed lasing action in the visible (red). While attempts at NSLS continue, Madey has obtained Department of Defense (DOD) funding to build a 1-GeV storage ring for FEL studies; the plans are to push the wavelength into the UV and XUV region and to increase the power in the visible. Because of the damage to mirrors by the accompanying x-ray SR, there are serious problems in going to the UV.

Calculations of the power and brightness of the radiation produced by storage-ring-based FELs are very impressive, and this radiation will certainly be more intense and brighter than the SR that can be produced in the UV. Thus, the net impact of FEL sources will significantly depend on how far into the XUV they can successfully achieve lasing.

Other concepts such as the transverse optical klystron also offer opportunities for producing UV laser radiation. It is unlikely that they will go above 100 eV. The storage ring designed for FEL use obviously can produce SR in the XUV region and as such is both complementary and supplementary to other activities. At Stanford, for example, the SR and FEL programs will share the new ring that is being built primarily for FEL development.

Because of the FEL's similarity to insertion devices, calling it an alternative source rather than another use of insertion devices in a storage ring is somewhat questionable. In any case, the development of FELs should certainly be pursued in both the infrared and the UV; their development is of course of great interest to the SR community. Hopefully, the new facility at Stanford will be made available as appropriate to the SR community.